

chain nodes:

7 9 10 11

ring nodes:

1 2 3 4 5 6

chain bonds:

4-7 7-10 7-9 10-11

ring bonds:

1-2 1-6 2-3 3-4 4-5 5-6

exact/norm bonds:

7-10 7-9 10-11

exact bonds:

4-7

normalized bonds:

1-2 1-6 2-3 3-4 4-5 5-6

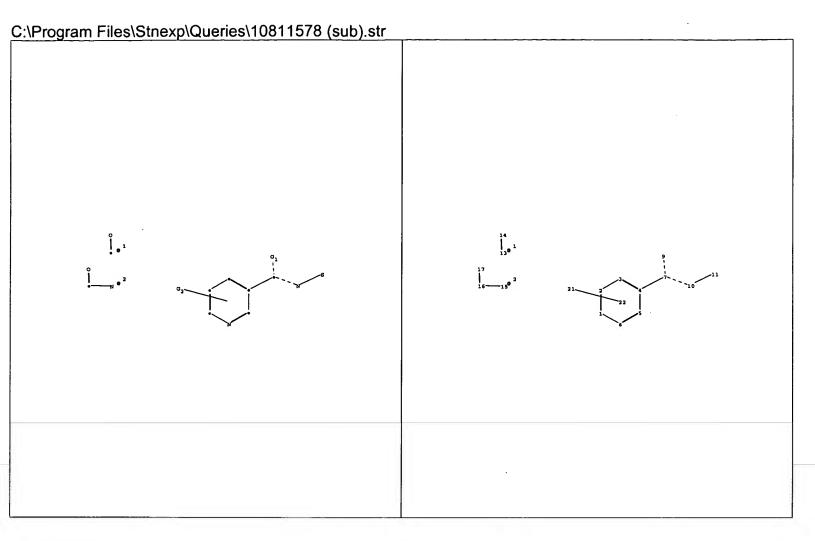
isolated ring systems:

containing 1:

G1:0,S

Match level:

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS9:CLASS10:CLASS11:CLASS



chain nodes:

7 9 10 11 13 14 15 16 17 21

ring nodes:

1 2 3 4 5 6

chain bonds:

4-7 7-10 7-9 10-11 13-14 15-16 16-17

ring bonds:

1-2 1-6 2-3 3-4 4-5 5-6

exact/norm bonds:

7-10 7-9 10-11 13-14 15-16 16-17

exact bonds:

4-7

normalized bonds:

1-2 1-6 2-3 3-4 4-5 5-6

isolated ring systems:

containing 1:

G1:0,S

G2:[*1],[*2]

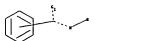
Match level:

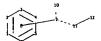
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS9:CLASS10:CLASS11:CLASS13:CLASS14:CLASS 15:CLASS

16:CLAS\$17:CLAS\$21:CLAS\$22:Atom

=>

Uploading C:\Program Files\Stnexp\Queries\10811578.str





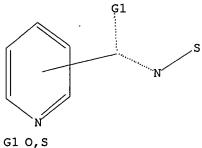
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chain nodes :
7  10  11  12
ring nodes :
1  2  3  4  5  6
chain bonds :
7-10  7-11  11-12
ring bonds :
1-2  1-6  2-3  3-4  4-5  5-6
exact/norm bonds :
7-10  7-11  11-12
normalized bonds :
1-2  1-6  2-3  3-4  4-5  5-6
isolated ring systems :
containing 1 :
```

G1:0,S

Match level:
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:Atom 10:CLASS 11:CLASS 12:CLASS

L1 STRUCTURE UPLOADED

=> d 11 L1 HAS NO ANSWERS L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l1 sss sam

SAMPLE SEARCH INITIATED 08:01:08 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 1541 TO ITERATE

100.0% PROCESSED 1541 ITERATIONS 45 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 28466 TO 33174
PROJECTED ANSWERS: 498 TO 1302

L2 45 SEA SSS SAM L1

=> =>

Uploading C:\Program Files\Stnexp\Queries\10811578 (a).str

```
7 9 10 11
ring nodes :
1 \quad \bar{2} \quad 3 \quad 4 \quad 5 \quad 6
chain bonds :
4-7 7-10 7-9 10-11
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
7-10 7-9 10-11
exact bonds :
4-7
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
containing 1:
G1:0,S
Match level:
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 9:CLASS 10:CLASS
11:CLASS
```

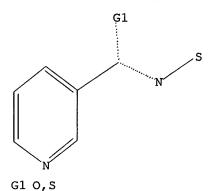
chain nodes :

L3 STRUCTURE UPLOADED

=> d 13

L3 HAS NO ANSWERS

L3 STR



Structure attributes must be viewed using STN Express query preparation.

=> s 13 sss sam

SAMPLE SEARCH INITIATED 08:07:01 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 90 TO ITERATE

100.0% PROCESSED 90 ITERATIONS 26 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 1231 TO 2369

PROJECTED ANSWERS: 215 TO 825

L4 26 SEA SSS SAM L3

=> => s 13 sss ful

FULL SEARCH INITIATED 08:10:18 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 1757 TO ITERATE

100.0% PROCESSED 1757 ITERATIONS 529 ANSWERS

SEARCH TIME: 00.00.01

L5 529 SEA SSS FUL L3

=>

Uploading C:\Program Files\Stnexp\Queries\10811578 (sub).str



```
chain nodes :
7 9 10 11 13 14 15 16 17 21
ring nodes :
1 2 3 4 5 6
chain bonds :
4-7 7-10 7-9 10-11 13-14 15-16 16-17
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
7-10 7-9 10-11 13-14 15-16 16-17
exact bonds :
4 - 7
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
containing 1 :
```

G1:0,S

G2:[*1],[*2]

Match level:

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 9:CLASS 10:CLASS 11:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 21:CLASS 22:Atom

L6 STRUCTURE UPLOADED

=> s 16 sub=15 sss sam
SAMPLE SUBSET SEARCH INITIATED 08:12:30 FILE 'REGISTRY'
SAMPLE SUBSET SCREEN SEARCH COMPLETED - 26 TO ITERATE

100.0% PROCESSED 26 ITERATIONS 13 ANSWERS

SEARCH TIME: 00.00.01

PROJECTIONS (WITHIN SPECIFIED SUBSET): ONLINE **COMPLETE**
PROJECTED ITERATIONS (WITHIN SPECIFIED SUBSET): 215 TO 825
PROJECTED ANSWERS (WITHIN SPECIFIED SUBSET): 44 TO 476

L7 13 SEA SUB=L5 SSS SAM L6

=> s 16 sub=15 sss ful FULL SUBSET SEARCH INITIATED 08:12:37 FILE 'REGISTRY' FULL SUBSET SCREEN SEARCH COMPLETED - 529 TO ITERATE

100.0% PROCESSED 529 ITERATIONS 156 ANSWERS

SEARCH TIME: 00.00.01

L8 156 SEA SUB=L5 SSS FUL L6

=> s 15 not 18 L9 373 L5 NOT L8

=> => s 19 L10 83 L9

=> d 110 1-83 bib, ab, hitstr

```
L10 ANSWER 1 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
     2006:579497 CAPLUS
AN
DN
     145:62925
TI
     Preparation of N-acylsulfonamide apoptosis promoters
IN
     Bruncko, Milan; Ding, Hong; Elmore, Steven; Kunzer, Aaron; Lynch,
     Christopher L.; Mcclellan, William; Park, Cheol-Min; Petros, Andrew; Song,
     Xiaohong; Wang, Xilu; Tu, Noah; Wendt, Michael
PA
SO
     U.S. Pat. Appl. Publ., 142 pp., Cont.-in-part of Ser. No. US 2004-988338,
     filed on 12 Nov 2004 which
     CODEN: USXXCO
DT
     Patent
LΑ
     English
FAN.CNT 3
     PATENT NO.
                         KIND
                                DATE
                                            APPLICATION NO.
                                                                    DATE
PΙ
     US 2006128706
                          A1
                                20060615
                                            US 2005-127940
                                                                    20050512
                                20050721
                                            US 2004-988338
     US 2005159427
                          A1
                                                                   20041112
PRAI US 2003-519695P
                          Ρ
                                20031113/
     US 2004-988338
                          A2
                                20041112
     Disclosed are N-acylsulfonamide compds. I [A1 = N, CA2; one or two or
AB
     three or each of A2, B1, D1 and E1 = R1, OR1, SR1, NHR1, etc., and the
     remainder = H, halo, CN, etc.; Y1 = H, CN, NO2, CO2H, etc.; or B1 and Y1,
     together with the atoms to which they are attached, = imidazole or
     triazole; one or two or each of A2, D1 and E1 = R1, OR1, SR1, etc., and
     the remainder = H, halo, CF3, etc.; R1 = Ph (un)fused with (hetero)arene,
     heteroaryl (un) fused with (hetero) arene, etc.; Z1 = substituted Ph
     (un) fused with (hetero) arene, heteroaryl (un) fused with (hetero) arene]
     which inhibit the activity of anti-apoptotic protein family members,
     compns. containing the compds. I and uses of the compds. I for preparing
     medicaments for treating diseases during which occurs expression of one or
     more than one anti-apoptotic protein family member. Over 460 synthetic
     examples were presented (no characterization data for intermediates).
     E.g., a multi-step synthesis of (1R)-II, starting from piperazine and Et
     4-fluorobenzoate, was given. The compds. I were found to be inhibitors of
     anti-apoptotic Bcl-XL protein and anti-apoptotic Bcl-2 (data given).
IT
     852810-24-3P 852810-28-7P 852810-29-8P
     RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
     (Uses)
        (preparation of N-acylsulfonamide apoptosis promoters)
RN
     852810-24-3 CAPLUS
CN
     3-Pyridinecarboxamide, 6-[4-[(4'-chloro[1,1'-biphenyl]-2-yl)methyl]-1-
     piperazinyl]-N-[[4-[[(1R)-3-(dimethylamino)-1-
     [(phenylthio)methyl]propyl]amino]-3-nitrophenyl]sulfonyl]- (9CI) (CA
     INDEX NAME)
```

PAGE 1-B

RN 852810-28-7 CAPLUS

CN 3-Pyridinecarboxamide, 6-[4-[(4'-chloro[1,1'-biphenyl]-2-yl)methyl]-1-piperazinyl]-N-[[4-[[(1R)-3-(4-morpholinyl)-1-[(phenylthio)methyl]propyl]amino]-3-nitrophenyl]sulfonyl]- (9CI) (CA INDEX NAME)

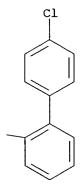
PAGE 1-B

RN 852810-29-8 CAPLUS

CN 3-Pyridinecarboxamide, 6-[4-[(4'-chloro[1,1'-biphenyl]-2-yl)methyl]-1-piperazinyl]-N-[[4-[[(1R)-3-(dimethylamino)-1-[(phenylthio)methyl]propyl]amino]-3-(trifluoromethyl)phenyl]sulfonyl]-(9CI) (CA INDEX NAME)

Me₂N
$$\stackrel{H}{\underset{\text{Phs}}}$$
 $\stackrel{H}{\underset{\text{F_3C}}}$ $\stackrel{N}{\underset{\text{O}}{\underset{\text{O}}{\text{O}}}}$ $\stackrel{N}{\underset{\text{O}}{\underset{\text{O}}{\text{O}}}}$

PAGE 1-B



```
T.10
     ANSWER 2 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
     2005:1216425 CAPLUS
ΑN
DN
     143:477970
TI
     Preparation of benzene derivatives containing amide moiety as ACC
     inhibitors
TN
     Suzuki, Nobuyasu; Nihei, Yukio; Ichinose, Hidehiro; Tanaka, Hideyuki;
     Yasa, Noriko; Hatanaka, Toshihiro; Masuzawa, Youko; Nakanishi, Eiji;
     Kondo, Nobuo
     Ajinomoto Co., Inc., Japan
PA
     PCT Int. Appl., 227 pp.
SO
     CODEN: PIXXD2
DT
     Patent
     Japanese
LΑ
FAN.CNT 1
                          KIND
                                  DATÈ.
                                              APPLICATION NO.
     PATENT NO.
                                                                       DATE
         2005108370 A1 20051117 WO 2005-JP7392 20050418
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
                                              WO 2005-JP7392
PI
     WO 2005108370
             CN, CO, CR, CU, ČZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
             GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ,
             LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA,
             NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL,
             SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA,
             ZM, ZW
         RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,
             AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,
             EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT,
             RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML,
             MR, NE, SN, TD, TG
PRAI JP 2004-122199
                                  20040416
                           Α
     JP 2004-122200
                           Α
                                  20040416
     JP 2004-122201
                                  20040416
                           Α
     JP 2005-21616
                           Α
                                  20050128
os
     MARPAT 143:477970
     Title compds. I [X = Q1, etc.; ring A = (un)substituted aromatic hydrocarbon,
AB
     (un) substituted aromatic heterocycle, (un) substituted cyclic alkenyl, etc.; B
     = single bond, -CO-, -NHCO-, etc.; R7 = (un) substituted alkyl,
     (un) substituted alkenyl, (un) substituted alkynyl, etc.; n = 0-5; V = Q2,
     etc.; R1-R3 = (un)substituted alkyl, (un)substituted alkenyl,
     (un) substituted alkynyl, etc.; R4-R6, R8 = (un) substituted alkyl,
     (un) substituted alkenyl, (un) substituted alkynyl, etc.] were prepared For
     example, amidation of compound II [R= OH], e.g., prepared from 4-nitrobenzoic acid in 4 steps, with anthranilic acid Et ester followed by hydrolysis
     using NaOH afforded compound II [R = 2-carboxyphenylamino]. In ACC (acetyl
     CoA carboxylase) inhibition assays, compound II [R = 2-carboxyphenylamino]
     exhibited the activity of 53%. Compds. I are claimed useful for the
     treatment of hyperlipidemia, diabetes, etc.
IT
     869577-82-2P
     RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
        (preparation of benzene derivs. containing amide moiety as ACC inhibitors
for
        treatment of hyperlipidemia, diabetes, etc.)
RN
     869577-82-2 CAPLUS
CN
     3-Pyridinecarboxamide, N-[[3-[3-[4-(2-phenyl-4-thiazolyl)phenyl]-1,2,4-
     oxadiazol-5-yl]phenyl]sulfonyl]- (9CI) (CA INDEX NAME)
```

RE.CNT 67 THERE ARE 67 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

```
L10
    ANSWER 3 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
     2005:1155549 CAPLUS
AN
DN
     143:405690
TI
     Preparation of phenoxyphenylacetamides as non-nucleoside reverse
     transcriptase inhibitors
     Dunn, James Patrick; Hirschfeld, Donald Roy; Silva, Tania; Sweeney,
IN
     Zachary Kevin; Vora, Harit
     Roche Palo Alto LLC, USA
PA
     U.S. Pat. Appl. Publ., 61 pp.
SO
     CODEN: USXXCO
DT
     Patent
     English
LΑ
FAN.CNT 2
                                ĎÁTÈ
     PATENT NO.
                         KIND
                                            APPLICATION NO.
                                                                    DATE
PΙ
     US 2005239881
                                120051027
                          A1
                                            US 2005-112591
                                                                    20050422
     WO 2005102989
                          A1
                                20051103
                                            WO 2005-EP4048
                                                                    20050415
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             GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ,
             LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA,
             NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL,
             SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA,
             ZM, ZW
         RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,
             AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,
             EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT,
             RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML,
             MR, NE, SN, TD, TG
PRAI US 2004-565117P
                          Ρ
                                20040423
    US 2004-565116P
                          P
                                20040423
OS
    MARPAT 143:405690
     Title compds. I [X1 = O; R1 and R2 independently = H, alkyl, haloalkyl,
ΑB
     etc. or together R1 and R2 are -O-CH=CH- or -O-CH2CH2- with provisions; R3
     and R4 independently = H, alkoxy, alkylthio, etc.; R5 = substituted aryl;
    Ar = substituted aryl] and their pharmaceutically acceptable salts, are
    prepared and disclosed as inhibitors of non-nucleoside reverse
     transcriptase. Thus, e.g., II was prepared by hydrolysis of III followed by
     chlorination and subsequent amidation using 4-amino-benzenesulfonamide.
     The inhibitory activity of I towards HIV1-RT was evaluated using
     radioactivity assay and it was revealed that selected compds. of the
     invention possessed IC50 values in the range of 0.0045 up to 0.027.
     inhibitor of non-nucleoside reverse transcriptase should prove useful in
     the treatment of HIV infection. Pharmaceutical compns. comprising I are
     disclosed.
TT
     867365-54-6P
     RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
        (preparation of phenoxyphenylacetamides as non-nucleoside reverse
        transcriptase inhibitors)
RN
     867365-54-6 CAPLUS
CN
     3-Pyridinecarboxamide, N-[[4-[[[4-chloro-3-(3-chloro-5-cyanophenoxy)-2-
     fluorophenyl]acetyl]amino]-3-methylphenyl]sulfonyl]-, monohydrochloride
           (CA INDEX NAME)
     (9CI)
```

$$\begin{array}{c|c} & & & \\ &$$

HCl

```
L10
     ANSWER 4 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
     2005:1155548 CAPLUS
AN
DN
     143:416204
     Use of phenylacetamides as non-nucleoside reverse transcriptase inhibitors
TI
     for treating retroviral infections
     Roche Palo Alto LLC, USA
PA
     U.S. Pat. Appl. Publ., 67 pp.
SO
     CODEN: USXXCO
DT
     Patent
LΑ
     English
FAN.CNT 2
                                  DATE
     PATENT NO.
                          KIND
                                              APPLICATION NO.
                                                                       DATE
                          ____
                                               -----
                                                                       _____
                                  20051027
PΙ
     US 2005239880
                           A1
                                              US 2005-112590
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     WO 2005102989
                           A1
                                              WO 2005-EP4048
                                                                       20050415
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             LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA,
             NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL,
             SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA,
             ZM, ZW
         RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,
             AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,
             EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT,
             RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML,
             MR, NE, SN, TD, TG
PRAI US 2004-565116P
                           Ρ
                                  20040423
     US 2004-565117P
                           Ρ
                                  20040423
os
     MARPAT 143:416204
ΑB
     Title compds. I [X1 = 0, S, CH2, C(0); R1 \text{ and } R2 \text{ independently} = H, alkyl,
     haloalkyl, etc. or together R1 and R2 are -O-CH:CH- or -O-CH2CH2- with
     provisions; R3 and R4 independently = H, alkoxy, alkylthio, etc.; R5 =
     alkyl, haloalkyl, cycloalkyl aryl or heteroaryl; Ar = (un)substituted aryl
     or heteroaryl; R6 = H, alkyl; addnl. details are given in the claims] and
     their pharmaceutically acceptable salts, are prepared and disclosed as
     inhibitors of non-nucleoside reverse transcriptase for use in treating or
     preventing an HIV infection, or treating AIDS or ARC. Although the
     methods of preparation are not claimed, .apprx.60 example prepns. are included.
     For example, II was prepared by hydrolysis of III followed by chlorination
     and subsequent amidation using 4-aminobenzenesulfonamide. The inhibitory
     activity of I towards HIV1-RT was evaluated using radioactivity assay and
     it was revealed that selected compds. of the invention possessed IC50
     values = 0.0045-0.027.
IT
     867365-54-6P
     RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
     (Uses)
        (use of phenylacetamides as non-nucleoside reverse transcriptase
        inhibitors for treating retroviral infections)
     867365-54-6 CAPLUS
CN
     3-Pyridinecarboxamide, N-[[4-[[[4-chloro-3-(3-chloro-5-cyanophenoxy)-2-
     fluorophenyl]acetyl]amino]-3-methylphenyl]sulfonyl]-, monohydrochloride
            (CA INDEX NAME)
```

• HCl

L10 ANSWER 5 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

AN 2005:480040 CAPLUS

DN 143:90225

TI Pharmacophore, Drug Metabolism, and Pharmacokinetics Models on Non-Peptide AT1, AT2, and AT1/AT2 Angiotensin FT Receptor Antagonists

AU Berellini, Giuliano; Cruciani, Gabriele; Mannhold, Raimund

CS Laboratory for Chemometrics and Cheminformatics, Department of Chemistry, University of Perugia, Perugia, I-06123, Italy

SO Journal of Medicinal Chemistry (2005), 48(13), 4389-4399 CODEN: JMCMAR; ISSN: 0022-2623

PB American Chemical Society

DT Journal

LA English

AΒ About 20 nonpeptide angiotensin II receptor antagonists are in various stages of clin. development. Different modeling approaches were used to predict the pharmacophoric requirements for AT1 (angiotensin II receptor subtype 1) affinity. However, to our knowledge, none was used to predict both the selectivity toward AT1 and AT2 (angiotensin II receptor subtype 2) receptor subtypes. In this paper, partial least squares discriminant anal. is applied to derive the chemical features guiding AT1 and AT2 selectivity or mixed AT1/AT2 receptor binding. The method can be used to modulate AT1 vs. AT2 selectivity. Concerns that unopposed stimulation of the AT2 receptor might produce adverse effects initiated a search for new balanced antagonists. Moreover, it can serve as a fast filtering procedure in database searches. Finally, some relevant pharmacokinetics and metabolic properties of the database of 53 compds. are calculated using the VolSurf and MetaSite software to allow the simultaneous characterization of pharmacodynamic and pharmacokinetics properties of the chemical space of angiotensin II receptor antagonists. IT

160632-48-4, L 735286
RL: PAC (Pharmacological activity); PKT (Pharmacokinetics); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (L 735286; pharmacophore, drug metabolism, and pharmacokinetics models on non-peptide AT1, AT2, and AT1/AT2 angiotensin II receptor antagonists)

RN 160632-48-4 CAPLUS

CN 3-Pyridinecarboxamide, N-[[4'-[(2-ethyl-4,6-dimethyl-1H-benzimidazol-1-yl)methyl][1,1'-biphenyl]-2-yl]sulfonyl]- (9CI) (CA INDEX NAME)

Me N Et
$$CH_2$$
 $O = S = O$ $C = NH$

RE.CNT 47 THERE ARE 47 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

```
ANSWER 6 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
L10
AN
     2005:472142 CAPLUS
     143:26639
DN
     Preparation of N-acylsulfonamide apoptosis promoters
ΤI
     Bruncko, Milan; Ding, Hong; Elmore, Steven; Kunzer, Aaron R.; Lynch,
IN
     Christopher L.; Mcclellan, William; Park, Cheol-Min; Petros, Andrew; Song,
     Xiaohong; Wang, Xilu; Tu, Noah; Wendt, Michael D.
PA
     Abbott Laboratories, USA
     PCT Int. Appl., 507 pp.
SO
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                           W
                                 20041112
os
     MARPAT 143:26639
AΒ
     Disclosed are N-acylsulfonamide compds. I [A1 = N, CA2; one or two or
     three or each of A2, B1, D1 and E1 = R1, OR1, SR1, NHR1, etc., and the
     remainder = H, halo, CN, etc.; Y1 = H, CN, NO2, CO2H, etc.; or B1 and Y1,
     together with the atoms to which they are attached, = imidazole or
     triazole; one or two or each of A2, D1 and E1 = R1, OR1, SR1, etc., and
     the remainder = H, halo, CF3, etc.; R1 = Ph (un)fused with (hetero)arene,
     heteroaryl (un) fused with (hetero) arene, etc.; Z1 = substituted Ph
     (un) fused with (hetero) arene, heteroaryl (un) fused with (hetero) arene]
     which inhibit the activity of anti-apoptotic protein family members,
     compns. containing the compds. I and uses of the compds. I for preparing
     medicaments for treating diseases during which occurs expression of one or
     more than one anti-apoptotic protein family member. Over 450 synthetic
     examples were presented (no characterization data for intermediates).
     E.g., a multi-step synthesis of (1R)-II, starting from piperazine and Et
     4-fluorobenzoate, was given. The compds. I were found to be inhibitors of
     anti-apoptotic Bcl-XL protein and anti-apoptotic Bcl-2 (data given).
IT
     852810-24-3P 852810-28-7P 852810-29-8P
     RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
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     (Uses)
        (preparation of N-acylsulfonamide apoptosis promoters)
     852810-24-3 CAPLUS
RN
CN
     3-Pyridinecarboxamide, 6-[4-[(4'-chloro[1,1'-biphenyl]-2-yl)methyl]-1-
     piperazinyl]-N-[[4-[[(1R)-3-(dimethylamino)-1-
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[(phenylthio)methyl]propyl]amino]-3-nitrophenyl]sulfonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

PAGE 1-B

RN 852810-28-7 CAPLUS

CN 3-Pyridinecarboxamide, 6-[4-[(4'-chloro[1,1'-biphenyl]-2-yl)methyl]-1-piperazinyl]-N-[[4-[((1R)-3-(4-morpholinyl)-1-[(phenylthio)methyl]propyl]amino]-3-nitrophenyl]sulfonyl]- (9CI) (CA INDEX NAME)

PAGE 1-B

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CN 3-Pyridinecarboxamide, 6-[4-[(4'-chloro[1,1'-biphenyl]-2-yl)methyl]-1-piperazinyl]-N-[[4-[((1R)-3-(dimethylamino)-1-[(phenylthio)methyl]propyl]amino]-3-(trifluoromethyl)phenyl]sulfonyl]-(9CI) (CA INDEX NAME)

PAGE 1-B

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ANSWER 7 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
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AN
     143:26638
DИ
     Preparation of N-acylsulfonamide apoptosis promoters
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     Bruncko, Milan; Elmore, Steven; Kunzer, Aaron R.; Lynch, Christopher L.;
IN
     Wang, Xilu; Wendt, Michael D.
PA
     Abbott Laboratories, USA
SO
     PCT Int. Appl., 471 pp.
     CODEN: PIXXD2
DT
     Patent
     English
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              NE, SN, TD, TG
PRAI US 2003-519695P
                                  20031113
     MARPAT 143:26638
OS
AB
     Disclosed are N-acylsulfonamide compds. I [A1 = N, CA2; one or two or
     three or each of A2, B1, D1 and E1 = R1, OR1, SR1, NHR1, etc., and the
     remainder = H, halo, CN, etc.; Y1 = H, CN, NO2, CO2H, etc.; or B1 and Y1,
     together with the atoms to which they are attached, = imidazole or
     triazole; one or two or each of A2, D1 and E1 = R1, OR1, SR1, etc., and
     the remainder = H, halo, CF3, etc.; R1 = Ph (un)fused with (hetero)arene,
     heteroaryl (un)fused with (hetero)arene, etc.; Z1 = substituted Ph
     (un) fused with (hetero) arene, heteroaryl (un) fused with (hetero) arene]
     which inhibit the activity of anti-apoptotic protein family members,
     compns. containing the compds. I and uses of the compds. I for preparing
     medicaments for treating diseases during which occurs expression of one or
     more than one anti-apoptotic protein family member. Over 440 synthetic
     examples were presented (no characterization data for intermediates).
     E.g., a multi-step synthesis of (1R)-II, starting from piperazine and Et
     4-fluorobenzoate, was given. The compds. I were found to be inhibitors of
     anti-apoptotic Bcl-XL protein and anti-apoptotic Bcl-2 (data given).
     852810-24-3P 852810-28-7P 852810-29-8P
IT
     RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
     (Uses)
         (preparation of N-acylsulfonamide apoptosis promoters)
RN
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     piperazinyl]-N-[[4-[[(1R)-3-(dimethylamino)-1-
     [(phenylthio)methyl]propyl]amino]-3-nitrophenyl]sulfonyl]- (9CI)
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PAGE 1-B

RN 852810-28-7 CAPLUS

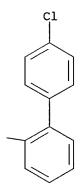
CN 3-Pyridinecarboxamide, 6-[4-[(4'-chloro[1,1'-biphenyl]-2-yl)methyl]-1-piperazinyl]-N-[[4-[[(1R)-3-(4-morpholinyl)-1-[(phenylthio)methyl]propyl]amino]-3-nitrophenyl]sulfonyl]- (9CI) (CA INDEX NAME)

PAGE 1-B

RN 852810-29-8 CAPLUS

CN 3-Pyridinecarboxamide, 6-[4-[(4'-chloro[1,1'-biphenyl]-2-yl)methyl]-1-piperazinyl]-N-[[4-[[(1R)-3-(dimethylamino)-1-[(phenylthio)methyl]propyl]amino]-3-(trifluoromethyl)phenyl]sulfonyl]-(9CI) (CA INDEX NAME)

PAGE 1-B



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     ANSWER 8 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
     2004:822772 CAPLUS
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     141:314166
DN
     Preparation of pyridinylcarboxamides and related compounds as herbicides
TT
     and pesticides
IN
     Schwarz, Hans-Georg; Bretschneider, Thomas; Konze, Joerg; Loesel, Peter;
     Drewes, Mark Wilhelm; Feucht, Dieter
PA
     Bayer Cropscience A.-G., Germany
     Ger. Offen., 41 pp.
SO
     CODEN: GWXXBX
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LA
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                                 20030326
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     Title compds. I [Y = (0)n; X = S(0)m; m = 0-2; n = 0,1; A = N, CH; O = O,
     S; R1 = (un)substituted alkyl; R2 = H, (un)substituted alkyl; R3 = H,
     (un) substituted alkyl; R4 = (un) substituted amino or alkyl with 2-carbon
     atoms with provisos] were prepared For example, N-acylation of
     N-cyanomethyl-3-chlorobenzensulfonamide with 4-(trifluoromethyl)nicotinoyl
     chloride afforded pyridinylcarboxamide II in 48% yield. In
    plant-protection assays against Myzus persicae, pyridinylcarboxamide II
     exhibited at 500 ppm application exhibited 100% Myzus mortality after
     6-days. Compds. I are claimed are suitable for the fight against
     vegetable and animal pests (sic).
IT
     769159-64-0P 769159-65-1P 769159-66-2P
     769159-67-3P 769159-68-4P 769159-69-5P
     RL: AGR (Agricultural use); BSU (Biological study, unclassified); SPN
     (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES
     (Uses)
        (preparation of pyridinylcarboxamides and related compds. as herbicides and
        pesticides)
RN
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     3-Pyridinecarboxamide, N-[(3-chlorophenyl)sulfonyl]-N-(cyanomethyl)-4-
     (trifluoromethyl) - (9CI) (CA INDEX NAME)
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RN 769159-65-1 CAPLUS

CN 3-Pyridinecarboxamide, N-(cyanomethyl)-N-[(3-methylphenyl)sulfonyl]-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 769159-66-2 CAPLUS

CN 3-Pyridinecarboxamide, N-(cyanomethyl)-N-[(3,4-dichlorophenyl)sulfonyl]-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 769159-67-3 CAPLUS

CN 3-Pyridinecarboxamide, N-(cyanomethyl)-N-[(4-methoxyphenyl)sulfonyl]-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 769159-68-4 CAPLUS

CN 3-Pyridinecarboxamide, N-(cyanomethyl)-N-[(4-phenoxyphenyl)sulfonyl]-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 769159-69-5 CAPLUS

CN 3-Pyridinecarboxamide, N-(cyanomethyl)-N-[(1,1-dimethylethyl)thio]-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

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ANSWER 9 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
AN
     2004:648518 CAPLUS
DN
     141:174066
     Preparation of (aryloxyalkyl) furans and related compounds as EP4 receptor
ΤI
     antagonists for treatment of migraines
     Clark, David Edward; Clark, Kenneth Lyle; Coleman, Robert Alexander;
IN
     Davis, Richard Jon; Fenton, Garry; Harris, Neil Victor; Hynd, George;
     Newton, Christoper Gregory; Oxford, Alexander William; Stuttle, Keith
     Alfred James; Sutton, Jonathan Mark
PA
     Pharmagene Laboratories Limited, UK
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     PCT Int. Appl., 176 pp.
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OS
     Title compds. I [wherein R2 = H, (un) substituted alkyl; Y = (CH2) nX, NRN1,
AB
     CONRN2; n = 1, 2; X = 0, S, SO, SO2; RN1 = H, (un) substituted alkyl; RN2 = H
     H, (un)substituted alkyl, aryl; R3 = (un)substituted aryl linked to an
     (un) substituted aryl group, wherein if both aryl groups are benzene rings,
     there may be an O bridge between the two rings; A = a single bond,
     alkylene; R5 = carboxy, CONHSO2R, SO2NHCOR, tetrazol-5-yl; R =
     (un) substituted alkyl, aryl, NRN3RN4; RN3 and RN4 = independently
     (un) substituted alkyl; and pharmaceutically acceptable salts thereof] were
     prepared as prostaglandin EP4 receptor antagonists. For example,
     (2-methylfuran-3-yl)methanol was coupled with tert-butyldiphenylsilyl
     chloride in the presence imidazole in DMF to give the protected alc.,
     3-(tert-butyldiphenylsilanyloxymethyl)-2-methylfuran. Reaction of the
     furan with BuLi in THF, followed by addition of CO2 provided
     4-(tert-butyldiphenylsilanyloxymethyl)-5-methylfuran-2-carboxylic acid.
     The latter was loaded onto 2-chlorotrityl chloride resin swelled with
     CH2Cl2 using diisopropylethylamine, and the loaded resin treated with
     tetrabutylammonium fluoride in THF. The resin-bound alc. was coupled with
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4-hydroxy-4'-methoxybiphenyl using PPh3 and diisopropyl azodicarboxylate in THF and the acid cleaved with TFA /H2O to afford II. In binding assays

demonstrated selectivity for antagonizing EP4 receptors over EP3 and EP2

using cells stably transfected with human EP receptor cDNA, II

receptors (pKi = >6.5, <5, and <5, resp.). Thus, I and their

pharmaceutical compns. are useful for the treatment of conditions alleviated by antagonism of an EP4 receptor, such as primary headache disorder and migraine (no data).

736182-66-4P, 4-(Biphenyl-4-yloxymethyl)-5-methylfuran-2-sulfonic acid [(pyridin-3-yl)carbonyl]amide

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(EP4 receptor antagonist; preparation of (aryloxyalkyl) furans and related compds. as EP4 receptor antagonists for treatment of migraines)

RN 736182-66-4 CAPLUS

CN 3-Pyridinecarboxamide, N-[[4-[([1,1'-biphenyl]-4-yloxy)methyl]-5-methyl-2-furanyl]sulfonyl]- (9CI) (CA INDEX NAME)

10/811,578

- L10 ANSWER 10 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
- 2004:204617 CAPLUS AN
- DN 142:23213
- ΤI Product class 4: 1,4,2-oxathiazoles and related compounds
- AU
- Argyropoulos, N. G.
 Lab. of Organic Chemistry Dept. of Chemistry, Aristotle University of CS Thessaloniki, Thessaloniki, 540 06, Greece Science of Synthesis (2004), 13, 95-107
- SO
- CODEN: SSCYJ9
- Georg Thieme Verlad PΒ
- Journal; General Re∜iew DT
- LA English
- AΒ A review. Preparation of oxathiazole, dithiazole and their cationic hetarene salts is reported via ring closure, aromatization, solvolysis and substituent modification reactions.
- IT 138906-05-5P
 - RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 - (preparation of oxathiazole, dithiazole and their cationic hetarene salts)
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- CN 3-Pyridinecarboxamide, N-[[(dimethylamino)thioxomethyl]thio]- (9CI) (CA INDEX NAME)

RE.CNT 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

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ANSWER 11 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
L10
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     2004:80685 CAPLUS
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     Preparation of bicyclic piperidine derivatives as antagonists of the CCR1
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     Blumberg, Laura Cook; Brown, Matthew Frank; Hayward, Matthew Merrill;
IN
     Poss, Christopher Stanley
PA
     Pfizer Products Inc., USA
     PCT Int. Appl., 90 pp.
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AB
     The title compds. [I; a = 1-5; b = 0-4; c = 0-1; Q = alkyl; W = aryl,
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     (CH2) \times O(CH2) y (wherein x, y = 1-2); R5 = H, halo, alkyl, etc.; R6 = H,
     halo, alkyl, etc.], useful as potent and selective inhibitors of
     MIP-l\alpha(CCL3) binding to its receptor CCR1 found on inflammatory and
     immunomodulatory cells (preferably leukocytes and lymphocytes), were
     prepared E.g., a multi-step synthesis of (trans)-5-chloro-2-{2-[3-(4-
     fluorophenoxy)-8-aza-bicyclo[3.2.1]oct-8-y1]-2-oxoethoxy}benzamide was
     given. All exemplified compds. I had IC50 of <10~\mu M in the chemotaxis
     assay. Pharmaceutical composition comprising the compound I is claimed.
IT
     652147-69-8P
     RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
        (preparation of bicyclic piperidine derivs. as antagonists of the CCR1
        chemokine receptor)
RN
     652147-69-8 CAPLUS
     3-Pyridinecarboxamide, 5-chloro-2-[[2-[(3-exo)-3-(4-fluorophenoxy)-8-
CN
     azabicyclo[3.2.1]oct-8-yl]-2-oxoethyl]amino]-N-(methylsulfonyl)-, rel-
```

(9CI) (CA INDEX NAME)

Relative stereochemistry.

RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

```
L10
     ANSWER 12 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
     2003:837072 CAPLUS
AN
     139:337887
DN
TI
     Preparation of heterocyclic amide derivatives as cytokine inhibitors
IN
     Gao, Donghong Amy; Goldberg, Daniel R.; Hammach, Abdelhakim; Hao,
     Ming-Hong; Moss, Neil; Qian, Kevin Chungeng; Roth, Gregory Paul; Sarko,
     Christopher Ronald; Swinamer, Alan David; Xiong, Zhaoming; Kamhi, Victor
PA
     Boehringer Ingelheim Pharmaceuticals, Inc., USA
SO
     PCT Int. Appl., 96 pp.
     CODEN: PIXXD2
DT
     Patent
LΑ
     English
FAN.CNT 1
     PATENT NO.
                         KIND
                                DATE
                                            APPLICATION NO.
                                                                    DATE
     WO 2003087085
PΙ
                          Α1
                                20031023
                                            WO 2003-US11094
                                                                    20030410
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         W: AE, AG, AL, AM, AT, AU, AZ,
             CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
             GM, HR, HU, ID, IL, IN, YS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
             LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM,
             PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT,
             TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
             KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES,
             FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR,
             BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
     CA 2478232
                          AΑ
                                20031023
                                            CA 2003-2478232
                                                                    20030410
    AU 2003224923
                          A1
                                20031027
                                            AU 2003-224923
                                                                    20030410
    US 2003225053
                          Α1
                                20031204
                                            US 2003-410688
                                                                    20030410
     EP 1497278
                          A1
                                20050119
                                            EP 2003-721619
                                                                    20030410
             AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK
     JP 2005530730
                          T2
                                20051013
                                            JP 2003-584041
                                                                    20030410
PRAI US 2002-371671P
                          Ρ
                                20020411
     WO 2003-US11094
                                20030410
                          W
    MARPAT 139:337887
AΒ
     Amides I [Q = N, (un)substituted CH; Y = (un)substituted CH2, CH:CH, O,
    NH, S, S(O), SO2; Ar = (un)substituted carbocyclic; R1, R4 = H, halogen,
     OH, CN, (un)substituted alkyl, alkenyl, alkynyl, NH2, alkoxy, alkylthio,
     acyl, alkoxycarbonyl, acyloxy; R2, R3 = H, alkyl, halogen] were prepared as
     inhibitors of the production of cytokines involved in inflammatory processes
     and are thus useful for treating diseases and pathol. conditions involving
     inflammation such as chronic inflammatory disease (no data). Thus, the
     amide II was prepared from 2-chloro-3-nitrobenzoic acid in 8 steps.
ΙT
     616238-77-8P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation of heterocyclic amide derivs. as cytokine inhibitors)
RN
     616238-77-8 CAPLUS
     3-Pyridinecarboxamide, 6-chloro-N-[3-[[[7-[[(6-chloro-3-
CN
     pyridinyl)carbonyl]amino]benzo[b]thien-2-yl]carbonyl]amino]-5-(1,1-
     dimethylethyl)-2-methoxyphenyl]-N-(methylsulfonyl)- (9CI) (CA INDEX NAME)
```

RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

```
L10
     ANSWER 13 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
     2003:282278 CAPLUS
AN
     138:282805
DN
     Preparation of N-thionicotinamide derivatives as pesticides
TI
IN
     Beckmann, Marion; Ort, Oswald; Doeller, Uwe; Krautstrunk, Gerhard;
     Schaper, Wolfgang; Luemmen, Peter; Jans, Daniela; Hempel, Waltraud;
     Waibel, Jutta Maria; Loerkens, Barbara
PA
     Bayer CropScience GmbH, Germany; et al.
SO
     PCT Int. Appl., 73 pp.
     CODEN: PIXXD2
DT
     Patent
T.A
     German
FAN.CNT 1
     PATENT NO.
                                  DATE
                          KIND
                                              APPLICATION NO.
                                                                       DATE
     _____
                          ____
                                  -----
                                              -----
ΡI
     WO 2003028458
                           A1
                                  20030410
                                              WO 2002-EP10279
                                                                       20020913
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             DM, DZ, EC, GD, GE, HR, HU, ID, IL, IN, IS, JP, KG, KP, KR, KZ, LC, LK, LR, LT, LV, MA, MD, MG, MK, MN, MX, NO, NZ, OM, PH, PL,
         RO, RU, SG, SI, TJ, TM, TN, TT, UA, US, UZ, VC, VN, YU, ZA
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
             KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES,
             FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF,
             CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
     DE 10146873
                           A1
                                  20030417
                                              DE 2001-10146873
                                                                       20010924
                                  20040630
     EP 1432313
                           A1
                                              EP 2002-762475
                                                                       20020913
         R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK
                                              JP 2003-531811
US 2002-246220
     JP 2005504104
                           Т2
                                  20050210
                                                                       20020913
     US 2003119852
                           A1
                                  20030626
                                                                       20020918
     US 2004192712
                           Α1
                                  20040930
                                              US 2004-811578
                                                                       20040329
PRAI DE 2001-10146873
                           Α
                                  20010924
     WO 2002-EP10279
                           W
                                  20020913
     US 2002-246220
                           B1
                                  20020918
os
     MARPAT 138:282805
AΒ
     The N-thionicotinamide derivs. I and II [X = CH or N; Y = O or S; n = 0 or
     1; m = n or 2; R1 = halo, (halo)alkyl, etc.; R2, R3 = H, halo,
     (halo)alkyl, etc.; R4 = H, un(substituted) (cyclo)alkyl, alkenyl, alkynyl
     aryl, heterocyclyl or alkanoyl; R5 = H, (un)substituted alkyl, alkenyl,
     alkynyl. etc. R6 = H, (un)substituted (cyclo)alkyl, etc.] are prepared as
     insecticides, acaricides and veterinary parasiticides.
IT
     506427-13-0P 506427-15-2P 506427-16-3P
     506427-18-5P 506427-19-6P 506427-20-9P
     506427-21-0P 506427-22-1P 506427-23-2P
     506427-24-3P 506427-25-4P 506427-26-5P
     506427-27-6P 506427-28-7P 506427-29-8P
     506427-30-1P 506427-31-2P 506427-32-3P
     506427-33-4P 506427-34-5P 506427-35-6P
     506427-36-7P 506427-37-8P 506427-38-9P
     506427-39-0P
     RL: AGR (Agricultural use); SPN (Synthetic preparation); THU (Therapeutic
     use); BIOL (Biological study); PREP (Preparation); USES (Uses)
        (preparation as pesticide)
RN
     506427-13-0 CAPLUS
     3-Pyridinecarboxamide, N-(cyclohexylthio)-4-(trifluoromethyl)- (9CI)
CN
     INDEX NAME)
```

Eveted species

RN 506427-15-2 CAPLUS

CN 3-Pyridinecarboxamide, N-[(1-methylpropyl)thio]-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 506427-16-3 CAPLUS

CN 3-Pyridinecarboximidic acid, N-[(1-methylethyl)thio]-4-(trifluoromethyl)-, butyl ester (9CI) (CA INDEX NAME)

RN 506427-18-5 CAPLUS

CN 3-Pyridinecarboxamide, N-butyl-N-[(1-methylethyl)thio]-4-(trifluoromethyl)-(9CI) (CA INDEX NAME)

RN 506427-19-6 CAPLUS

CN 3-Pyridinecarboxamide, N-cyclohexyl-N-[(phenylmethyl)thio]-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 506427-20-9 CAPLUS

CN 3-Pyridinecarboxamide, N-(cyclopentylthio)-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 506427-21-0 CAPLUS

CN 3-Pyridinecarboxamide, N-(phenylthio)-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 506427-22-1 CAPLUS

CN 3-Pyridinecarboxamide, N-ethyl-N-(phenylthio)-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 506427-23-2 CAPLUS

CN 3-Pyridinecarboxamide, N-(1-methylethyl)-N-(phenylthio)-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 506427-24-3 CAPLUS

CN 3-Pyridinecarboxamide, N-(1-methylethyl)-N-[(4-methylphenyl)thio]-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 506427-25-4 CAPLUS

CN 3-Pyridinecarboxamide, N-[(4-chlorophenyl)thio]-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 506427-26-5 CAPLUS

CN 3-Pyridinecarboxamide, N-[(4-fluorophenyl)thio]-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 506427-27-6 CAPLUS

CN 3-Pyridinecarboxamide, N-[(2-methylbutyl)thio]-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{Me} & \text{O} \\ \mid & \text{H} \\ \text{Et-CH-CH}_2\text{-S-NH-C} \\ & \text{F}_3\text{C} \end{array}$$

RN 506427-28-7 CAPLUS

CN 3-Pyridinecarboxamide, N-(2-propenylthio)-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

$$H_2C = CH - CH_2 - S - NH - C$$
 F_3C

RN 506427-29-8 CAPLUS

CN 3-Pyridinecarboxamide, N-[(3-methylbutyl)thio]-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

$$Me_2CH-CH_2-CH_2-S-NH-C$$

RN 506427-30-1 CAPLUS

CN 3-Pyridinecarboxamide, N-(pentylthio)-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Me- (CH₂)₄-s-NH-C
$$F_{3}$$
C

RN 506427-31-2 CAPLUS

CN 3-Pyridinecarboxamide, N-(hexylthio)-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Me- (CH₂)₅-s-NH-C
$$F_{3}C$$

RN 506427-32-3 CAPLUS

CN 3-Pyridinecarboxamide, N-(heptylthio)-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Me- (CH₂)₆-s-NH-C
$$F_{3}C$$

RN 506427-33-4 CAPLUS

CN 3-Pyridinecarboxamide, 4-(trifluoromethyl)-N-[[[4-(trifluoromethyl)phenyl]methyl]thio]- (9CI) (CA INDEX NAME)

RN 506427-34-5 CAPLUS

CN 3-Pyridinecarboxamide, 4-(trifluoromethyl)-N-[[[3-(trifluoromethyl)phenyl]methyl]thio]-(9CI) (CA INDEX NAME)

RN 506427-35-6 CAPLUS

CN 3-Pyridinecarboxamide, N-[(2-thienylmethyl)thio]-4-(trifluoromethyl)-(9CI) (CA INDEX NAME)

RN 506427-36-7 CAPLUS

CN 3-Pyridinecarboxamide, N-(cyclopropylthio)-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 506427-37-8 CAPLUS

CN 3-Pyridinecarboxamide, 2,6-dichloro-N-[(2-nitrophenyl)thio]-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 506427-38-9 CAPLUS

CN 3-Pyridinecarboxamide, 4-(trifluoromethyl)-N-[[2-(trimethylsilyl)ethyl]thio]-(9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me}_{3}\text{Si-CH}_{2}\text{-CH}_{2}\text{-S-NH-C} \\ \\ \text{F}_{3}\text{C} \end{array}$$

RN 506427-39-0 CAPLUS

CN 3-Pyridinecarboxamide, N-[(2-furanylmethyl)thio]-4-(trifluoromethyl)-(9CI) (CA INDEX NAME)

IT 506427-17-4

RL: RCT (Reactant); RACT (Reactant or reagent) (reactant in preparation of N-thionicotinamide pesticide)

RN 506427-17-4 CAPLUS

CN 3-Pyridinecarboxamide, N-[(1-methylethyl)thio]-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RE.CNT 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

```
L10
    ANSWER 14 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
     2003:221441 CAPLUS
AN
DN
     138:216842
TI
     Herbicide combinations with safeners
IN
     Ziemer, Frank; Willms, Lothar; Rosinger, Christopher; Bieringer, Hermann;
     Hacker, Erwin
PA
     Bayer CropScience GmbH, Germany
     PCT Int. Appl., 39 pp.
SO
     CODEN: PIXXD2
DT
     Patent
LΑ
     German
FAN.CNT 1
     PATENT NO.
                         KIND
                                DATE
                                            APPLICATION NO.
                                                                    DATE
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PΙ
     WO 2003022050
                          A1
                                20030320
                                            WO 2002-EP9973
                                                                    20020906
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             LC, LK, LR, LT, LV, MA, MD, MG, MK, MN, MX, NO, NZ, OM, PH, PL,
             RO, RU, SG, SI, TJ, TM, TN, TT, UA, US, UZ, VC, VN, YU, ZA
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG,
             CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL,
             PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR,
             NE, SN, TD, TG
     DE 10145019
                                20030403
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                                                                    20010913
     CA 2460481
                          AA
                                20030320
                                            CA 2002-2460481
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     EP 1427281
                          A1
                                20040616
                                            EP 2002-764874
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     BR 2002012488
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                                20040824
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     CN 1553769
                                20041208
                                            CN 2002-817899
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                                                                    20020906
     JP 2005501910
                                20050120
                                            JP 2003-526192
                          Т2
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     US 2003130120
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                                20030710
                                            US 2002-241136
                                                                    20020911
     US 6914035
                          B2
                                20050705
PRAI DE 2001-10145019
                          Α
                                20010913
     WO 2002-EP9973
                          W
                                20020906
OS
     MARPAT 138:216842
AB
     The invention concerns compns. containing an azole herbicide I [R = H or
     alkoxycarbonyl; R1 = H, (halo)alkyl, (halo)alkenyl, (halo)alkynyl,
     alkoxyalkyl, alkylthio, etc.; R2 = halo, nitro, cyano, (halo)alkyl,
     (halo)alkenyl, (halo)alkynyl, alkoxyalkyl, etc.; q = 0,1-4] and a safener
     II [X = CH or N; R3 = H, (un)substituted (cyclo)alkyl, (cyclo)alkenyl,
     alkynyl, Ph or heterocyclyl; R4 = H, (un)substituted alkyl, alkenyl or
     alkynyl; R3NR4 = pyrrolidinyl or piperidinyl; R5 = halo, nitro,
     (halo)alkyl, (halo)alkoxy, alkylsulfonyl, alkoxycarbonyl or alkylcarbonyl;
     R 6 = H alkyl, alkenyl or alkynyl; R7 = R5, cycloalkyl, Ph, cyano,
     alkylthio or alkylsulfinyl; s = 0,1 or 2; o = 1 or 2].
IT
     500905-91-9 500905-92-0
     RL: AGR (Agricultural use); BIOL (Biological study); USES (Uses)
        (safened herbicide)
     500905-91-9 CAPLUS
CN
     3-Pyridinecarboxamide, 2-methoxy-N-[[4-[[(1-methylethyl)amino]carbonyl]phe
     nyl]sulfonyl]-, mixt. with (5-cyclopropyl-4-isoxazolyl)[2-(methylsulfonyl)-
     4-(trifluoromethyl)phenyl]methanone (9CI) (CA INDEX NAME)
          1
     CM
     CRN
          221670-20-8
     CMF
          C17 H19 N3 O5 S
```

CM 2

CRN 141112-29-0 CMF C15 H12 F3 N O4 S

RN 500905-92-0 CAPLUS

CN 3-Pyridinecarboxamide, N-[[4-[(cyclopropylamino)carbonyl]phenyl]sulfonyl]-2-methoxy-, mixt. with (5-cyclopropyl-4-isoxazolyl)[2-(methylsulfonyl)-4-(trifluoromethyl)phenyl]methanone (9CI) (CA INDEX NAME)

CM 1

CRN 221670-23-1 CMF C17 H17 N3 O5 S

CM 2

CRN 141112-29-0

CMF C15 H12 F3 N O4 S

RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

10/811,578

L10 ANSWER 15 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

AN 2003:20483 CAPLUS

DN 138:204805

TI Unusual Reaction of Chloramine-T with Araldoximes

AU Padmavathi, V.; Reddy, K. Venugopal; Padmaja, A.; Venugopalan, P.

CS Department of Chemistry, Sri Venkateswara University, Tirupathi, 517502, India

SO Journal of Organic Chemistry (2003) 68(4), 1567-1570 CODEN: JOCEAH; ISSN: 0022-3283

PB American Chemical Society

DT Journal

LA English

OS CASREACT 138:204805

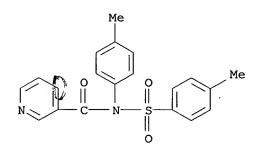
AB Reaction of araldoximes with 4 equiv of chloramine-T in refluxing methanol produces N-(p-tolyl)-N-(p-tosyl)benzamides via addition of 2 equiv of chloramine-T to the intermediate nitrile oxide followed by extrusion of sulfur dioxide.

IT 500362-82-3P RL: SPN (Synthetic prepa

RL: SPN (Synthetic preparation); PREP (Preparation)
 (reaction of chloramine-T with araldoximes)

RN 500362-82-3 CAPLUS

CN 3-Pyridinecarboxamide, N-(4-methylphenyl)-N-[(4-methylphenyl)sulfonyl]-(9CI) (CA INDEX NAME)



RE.CNT 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

```
ANSWER 16 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
L10
     2003:5781 CAPLUS
AN
DN
     138:73179
     Preparation of phenylvinyl-nicotinic acid derivatives for therapeutic use
ΤI
     glucokinase (GLK) activators
     Hayter, Barry Raymond; Currie, Gordon Stuart; Hargreaves, Rodney Brian;
IN
     Caulkett, Peter William Rodney; James, Roger
     Astrazeneca AB, Swed.; Astrazeneca UK Limited
PA
     PCT Int. Appl., 79 pp.
SO
     CODEN: PIXXD2
DT
     Patent
LА
     English
FAN.CNT 1
     PATENT NO.
                         KIND
                                DATE
                                            APPLICATION NO.
                                                                   DATE
                         ----
                                            ______
    WO 2003000262
                                20030103
                                            WO 2002-GB2903
PΙ
                         A1
                                                                   20020624
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             GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
             LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,
             PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ,
             UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU,
             TJ, TM
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH,
             CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR,
             BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
     EP 1406620
                          A1
                                20040414
                                           EP 2002-743377
                                                                   20020624
            AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO, MK, CY, AL, TR
     JP 2005500311
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                                20050106
                                           JP 2003-506907
                                                                   20020624
     US 2005054715
                                20050310
                                            US 2004-482264
                          Α1
                                                                   20040806
PRAI SE 2001-2299
                          Α
                                20010626
                                20020624
     WO 2002-GB2903
os
     MARPAT 138:73179
AB
     Phenylvinyl-nicotinic acid derivs., such as I [R1 = OH, (CH2)1-4OH, NO2,
     NH2, haloalkyl, haloalkyloxy, alkyl, alkenyl, alkylamino, etc.; R2 = X-Y;
    X = linking group, such as O, CO, amino, Z-O-Z, etc; Z = alkylene,
     alkenylene, etc.; R3 = OH, alkoxy, alkylamino, etc.; m = 0-2; n = 0-4; m + 1
     n > 0], as well as other phenylvinyl-heteroaryl derivs., were prepared for
     pharmaceutical use in the treatment of diseases or conditions mediated
     through glucokinase (GLK), such as type 2 diabetes. Thus, nicotinic acid
     derivative II (R3 = OH) was prepared via condensation of Me 6-methylnicotinate
     with PhO-3-C6H4CHO using AcOH at 120° for 24 h to give the
     corresponding Me ester II (R3 = OMe) in 49% yield, followed by hydrolysis
     of the ester using 1M aqueous NaOH in THF to give the desired acid in 76%
            The prepared compds. were assayed for their effect on GLK activity,
     and pharmaceutical compns. of the prepared compds. were presented.
IT
    ·479723-33-6P
     RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
        (preparation of phenylvinyl-nicotinic acid derivs. for therapeutic use
        glucokinase (GLK) activators)
RN
     479723-33-6 CAPLUS
CN
     3-Pyridinecarboxamide, N-(methylsulfonyl)-6-[(1E)-2-[5-(methylthio)-2-
    (phenylmethoxy)phenyl]ethenyl]- (9CI) (CA INDEX NAME)
```

Double bond geometry as shown.

RE.CNT 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

10/811,578

L10 ANSWER 17 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

AN 2002:728847 CAPLUS

DN 137:257628

TI Antitumor agents containing novel chroman derivatives

IN Fujita, Takashi; Wada, Kunio; Oguchi, Minoru; Kurakata, Shinichi

PA Sankyo Co., Ltd., Japan

SO Jpn. Kokai Tokkyo Koho, 101 pp.

CODEN: JKXXAF

DT Patent

LA Japanese

FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE		
PI JP 2002275064	A2	20020925	JP 2002-5560	20020115		
PRAI JP 2001-6574	Α	20010115				

OS MARPAT 137:257628

AB The invention provides chroman derivs. I (R1 = H, C1-6 alkyl, etc.; R2 = H, C1-6 alkyl, etc.; R3, R4, R5, R6 = H, C1-6 alkyl, etc.; X = single bond, CO, C:NOR7, etc.; R7, R8 = H, C1-6 alkyl, C2-6 alkenyl, etc.; A = CO, SO2; U = CH2, etc.; Y = O, S; Q = H, nitro, OH, etc.; k = 1-6; m, n = 0-8; Ar1 = benzene ring, etc.; Ar2 = benzene ring, etc.) as antitumor agents. The antitumor effect of N-[2-[4-(6-acetoxy-4-oxo-2,5,7,8-tetramethylchroman-2-ylmethoxy)phenyl]ethyl]-nicotinamide in SK-N-MC and D283-Med cells was examined Also, a capsule containing

N-[4-(6-acetoxy-2,5,7,8-

tetramethylchroman-2-ylmethoxy)phenyl]-nicotinamide 100 mg was prepared

IT 321919-68-0P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(chroman derivs. as antitumor agents)

RN 321919-68-0 CAPLUS

CN 3-Pyridinecarboxamide, N-[4-[[6-(acetyloxy)-3,4-dihydro-2,5,7,8-tetramethyl-2H-1-benzopyran-2-yl]methoxy]-3-(trifluoromethyl)phenyl]-N[(chloromethyl)sulfonyl]- (9CI) (CA INDEX NAME)

Me Me
$$F_3C$$
 $O=S-CH_2C1$ $N=CH_2C1$ $N=CH_$

grovino

```
ANSWER 18 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
AN
     2002:505411 CAPLUS
DN
     137:78769
TΙ
     Preparation of N-arylcarbonyl- and heteroarylcarbonyl benzenesulfonamide
     inhibitors of Bcl-Xl and Bcl-2 as promoters of apoptosis
IN
     Augeri, David J.; Baumeister, Steven A.; Bruncko, Milan; Dickman, Daniel
     A.; Ding, Hong; Dinges, Jurgen; Fesik, Stephen W.; Hajduk, Philip J.;
     Kunzer, Aaron R.; McClellan, William; Nettesheim, David G.; Oost,
     Thorsten; Petros, Andrew M.; Rosenberg, Saul H.; Wang, Shen; Thomas,
     Sheela A.; Wang, Xilu; Wendt, Michael D.
PA
     Abbott Laboratories, USA
     U.S. Pat. Appl. Publ., 126 pp.
SO
     CODEN: USXXCO
DT
     Patent
LA
     English
FAN.CNT 1
                                          APPLICATION NO.
                       KIND DATE
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                                                                  DATE
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                                -----
                    A1
B2
     US 2002086887
PΙ
                        A1 20020704 US 2001-957276
B2 20040413
A1 20040930 US 2004-820097
                                20020704
                                            US 2001-957276 20010920
     US 6720338
     US 2004192681
                                                                   20040407
PRAI US 2000-233866P P US 2001-957276 A3
                                20000920
                                20010920
OS
```

MARPAT 137:78769 AB N-aryl- and N-heteroarylcarbonyl benzenesulfonamides I [A = (un) substituted Ph, 5- or 6-membered heterocyclic ring with 1-3 N, O, or S atoms; R1 = alkyl, haloalkyl, NO2, NR6R7; R2, R3 = H, alkyl, alkenyl, alkynyl, alkoxy, alkylthio, etc.; R4 = aryl, arylalkenyl, arylalkoxy, cycloalkenyl, cycloalkyl, halo, heterocyclyl, heterocyclyloxy; R5 = H, alkyl, halo; R6, R7 = H, alkenyl, alkoxyalkyl, alkoxycarbonylalkyl, alkyl, heterocyclyl, etc.; R6R7N = imidazolyl, morpholinyl, piperazinyl, piperidinyl, pyrrolidinyl, etc.] are prepared Over 500 I are prepared E.g., N-biphenylcarbonyl benzenesulfonamide II was prepared by Pd-catalyzed coupling of 4-FC6H4B(OH)2 and 4-BrC6H4CO2Me, hydrolysis of the ester with LiOH, acylation of 4-chloro-3-nitrobenzenesulfonamide with the resulting acid in the presence of EDCI and DMAP, and nucleophilic aromatic substitution of the chlorobenzenesulfonamide with 2,2-dimethylcyclopentylamine. Compds. of the invention inhibit Bcl-Xl with IC50 values between 0.011 μM and 10 μM , and inhibit Bcl-2 with IC50 values between 0.017 μM and 10 μ M.

IT 406230-32-8P 406230-66-8P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of N-aryl- and heteroarylcarbonyl benzenesulfonamide inhibitors of Bcl-Xl and Bcl-2 as promoters of apoptosis)

RN 406230-32-8 CAPLUS

CN 3-Pyridinecarboxamide, N-[[4-[[(1R)-5-amino-1-[(phenylthio)methyl]pentyl]amino]-3-nitrophenyl]sulfonyl]-6-(4-fluorophenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PhS
$$(CH_2)_4$$
 R $(CH_2)_4$ R

RN 406230-66-8 CAPLUS

CN 3-Pyridinecarboxamide, 6-(4-fluorophenyl)-N-[[3-nitro-4-[[2-(phenylthio)ethyl]amino]phenyl]sulfonyl]- (9CI) (CA INDEX NAME)

RE.CNT 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

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ANSWER 19 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
     2002:354097 CAPLUS
AN
DN
     136:355074
TI
     Preparation of N-arylcarbonyl- and heteroarylcarbonyl benzenesulfonamide
     inhibitors of Bcl-Xl and Bcl-2 as promoters of apoptosis
     Augeri, David J.; Baumeister, Steven A.; Bruncko, Milan; Dickman, Daniel
IN
     A.; Ding, Hong; Dinges, Jurgen; Fesik, Stephen W.; Hajduk, Philip J.;
     Kunzer, Aaron R.; McClellan, William; Nettesheim, David G.; Oost,
     Thorsten; Petros, Andrew M.; Rosenberg, Saul H.; Shen, Wang; Thomas,
     Sheela A.; Wang, Xilu; Wendt, Michael D.
     Abbott Laboratories, USA
PA
SO
     U.S. Pat. Appl. Publ., 126 pp., Cont.-in-part of U.S. Ser. No. 666,508.
     CODEN: USXXCO
DT
     Patent
LА
     English
FAN.CNT 2
     PATENT NO.
                         KIND
                                 DATE
                                             APPLICATION NO.
                                                                     DATE
                         ____
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     US 2002055631
                                 20020509
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                                 20020328
                                             CA 2001-2423103
                                                                     20010920
     WO 2002024636
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                                 20020328
                                             WO 2001-US29432
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     WO 2002024636
                          A3
                                 20020926
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             CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
             GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
             LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL,
             PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG,
             UZ, VN, YU, ZA, ZW
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,
             DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF,
             BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
     AU 2001091151
                                 20020402
                                            AU 2001-91151
                          Α5
                                                                     20010920
     EP 1318978
                          A2
                                 20030618
                                             EP 2001-971244
                                                                     20010920
     EP 1318978
                                 20060208
                          В1
            AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO, MK, CY, AL, TR
     JP 2004529852
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                                 20040930
                                             JP 2002-529049
                                                                     20010920
     BR 2001010101
                          Α
                                 20050607
                                             BR 2001-10101
                                                                     20010920
     AT 317382
                          Е
                                 20060215
                                             AT 2001-971244
                                                                     20010920
PRAI US 2000-666508
                          A2
                                 20000920
     US 2001-935581
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                                 20010824
     WO 2001-US29432
                                20010920
OS
     MARPAT 136:355074
AΒ
     N-aryl- and N-heteroarylcarbonyl benzenesulfonamides I [A =
     (un) substituted Ph, 5- or 6-membered heterocyclic ring with 1-3 N, O, or S
     atoms; R1 = alkyl, haloalkyl, NO2, NR6R7; R2, R3 = H, alkyl, alkenyl,
     alkynyl, alkoxy, alkylthio, etc.; R4 = aryl, arylalkenyl, arylalkoxy,
     cycloalkenyl, cycloalkyl, halo, heterocyclyl, heterocyclyloxy; R5 = H,
     alkyl, halo; R6, R7 = H, alkenyl, alkoxyalkyl, alkoxycarbonylalkyl, alkyl,
     heterocyclyl, etc.; R6R7N = imidazolyl, morpholinyl, piperazinyl, piperidinyl, pyrrolidinyl, etc.] are prepared Over 500 I are prepared E.g.,
     N-biphenylcarbonyl benzenesulfonamide II was prepared by Pd-catalyzed
     coupling of 4-FC6H4B(OH)2 and 4-BrC6H4CO2Me, hydrolysis of the ester with
     LiOH, acylation of 4-chloro-3-nitrobenzenesulfonamide with the resulting
     acid in the presence of EDCI and DMAP, and nucleophilic aromatic substitution
     of the chlorobenzenesulfonamide with 2,2-dimethylcyclopentylamine.
```

Compds. of the invention inhibit Bcl-Xl with IC50 values between 0.011 μM and 10 μM , and inhibit Bcl-2 with IC50 values between 0.017 μM

Absolute stereochemistry.

RN 406230-66-8 CAPLUS

CN 3-Pyridinecarboxamide, 6-(4-fluorophenyl)-N-[[3-nitro-4-[[2-(phenylthio)ethyl]amino]phenyl]sulfonyl]- (9CI) (CA INDEX NAME)

10/811,578

L10 ANSWER 20 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

AN 2002:328512 CAPLUS

DN 138:89662

TI Synthesis and antibacterial activity of 2-(arylthioureido)-3-(p-toluenesulfonamidocarbonyl)pyridines

AU Patel, N. B.; Bhagat, P. R.

CS Department of Chemistry, South Gujarat University, Surat, 395007, India

SO Journal of Indian Council of Chemists (2001), 18(1), 56-58 CODEN: JICCE7; ISSN: 0971-5037

PB Indian Council of Chemists

DT Journal

LA English

OS CASREACT 138:89662

AB Title compds. I (R = H, 4-CO2H, 2-OMe, 4-OMe, 2-Me, 3-Me, 4-Me, etc.) were prepared from the 2-chloropyridine analogs and arylthioureas. Antibacterial activity screening for all I was carried out.

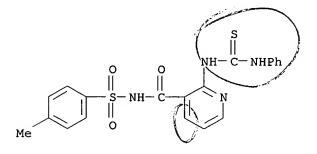
IT 484650-13-7P 484650-14-8P 484650-15-9P 484650-16-0P 484650-17-1P 484650-18-2P 484650-19-3P 484650-20-6P 484650-21-7P 484650-22-8P 484650-23-9P 484650-24-0P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(preparation and antibacterial activity of 2-(arylthioureido)-3-(p-toluenesulfonamidocarbonyl)pyridines)

RN 484650-13-7 CAPLUS

CN 3-Pyridinecarboxamide, N-[(4-methylphenyl)sulfonyl]-2-[[(phenylamino)thioxomethyl]amino]- (9CI) (CA INDEX NAME)



2 54

RN 484650-14-8 CAPLUS

CN Benzoic acid, 4-[[[[3-[[[(4-methylphenyl)sulfonyl]amino]carbonyl]-2-pyridinyl]amino]thioxomethyl]amino]- (9CI) (CA INDEX NAME)

RN 484650-15-9 CAPLUS

CN 3-Pyridinecarboxamide, 2-[[[(2-methoxyphenyl)amino]thioxomethyl]amino]-N-[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)

RN 484650-16-0 CAPLUS

CN 3-Pyridinecarboxamide, 2-[[[(4-methoxyphenyl)amino]thioxomethyl]amino]-N-[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)

RN 484650-17-1 CAPLUS

CN 3-Pyridinecarboxamide, 2-[[[(2-methylphenyl)amino]thioxomethyl]amino]-N-[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)

RN 484650-18-2 CAPLUS

CN 3-Pyridinecarboxamide, 2-[[[(3-methylphenyl)amino]thioxomethyl]amino]-N-[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)

RN 484650-19-3 CAPLUS

CN 3-Pyridinecarboxamide, 2-[[[(4-methylphenyl)amino]thioxomethyl]amino]-N-[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)

RN 484650-20-6 CAPLUS

CN 3-Pyridinecarboxamide, N-[(4-methylphenyl)sulfonyl]-2-[[[(2-nitrophenyl)amino]thioxomethyl]amino]- (9CI) (CA INDEX NAME)

RN 484650-21-7 CAPLUS

CN 3-Pyridinecarboxamide, N-[(4-methylphenyl)sulfonyl]-2-[[[(3-nitrophenyl)amino]thioxomethyl]amino]- (9CI) (CA INDEX NAME)

RN 484650-22-8 CAPLUS

CN 3-Pyridinecarboxamide, N-[(4-methylphenyl)sulfonyl]-2-[[[(4-nitrophenyl)amino]thioxomethyl]amino]- (9CI) (CA INDEX NAME)

RN 484650-23-9 CAPLUS

CN 3-Pyridinecarboxamide, 2-[[[(3-chlorophenyl)amino]thioxomethyl]amino]-N[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)

RN 484650-24-0 CAPLUS

CN 3-Pyridinecarboxamide, 2-[[[(4-chlorophenyl)amino]thioxomethyl]amino]-N-[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)

IT 113513-63-6

RL: RCT (Reactant); RACT (Reactant or reagent) (preparation and antibacterial activity of 2-(arylthioureido)-3-(p-toluenesulfonamidocarbonyl)pyridines)

RN 113513-63-6 CAPLUS

CN 3-Pyridinecarboxamide, 2-chloro-N-[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)

RE.CNT 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

```
L10
     ANSWER 21 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
     2002:240717 CAPLUS
ΑN
     136:279215
DN
     Preparation of N-arylcarbonyl- and heteroarylcarbonyl benzenesulfonamide
ΤI
     inhibitors of Bcl-Xl and Bcl-2 as promoters of apoptosis
     McClellan, William; Oost, Thorsten; Bruncko, Milan; Wang, Xilu; Augeri,
IN
     David J.; Baumeister, Steven A.; Dickman, Daniel A.; Ding, Hong; Dinges,
     Jurgen; Fesik, Stephen W.; Hajduk, Philip J.; Kunzer, Aaron R.;
     Nettesheim, David G.; Petros, Andrew M.; Rosenberg, Saul H.; Shen, Wang;
     Thomas, Sheela A.; Wendt, Michael D.
PA
     Abbott Laboratories, USA
     PCT Int. Appl., 292 pp.
SO
     CODEN: PIXXD2
DT
     Patent
LA
     English
FAN.CNT 2
     PATENT NO.
                         KIND
                                DATE
                                            APPLICATION NO.
                                                                    DATE
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PI
     WO 2002024636
                          A2
                                20020328
                                            WO 2001-US29432
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     WO 2002024636
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                                20020926
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             CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
             GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
             LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL,
             PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG,
         UZ, VN, YU, ZA, ZW
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,
             DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF,
             BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
     US 2002055631
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                                                                    20010824
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                          В1
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            AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
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     JP 2004529852
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                                20040930
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PRAI US 2000-666508
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                          Α
     US 2001-935581
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                                20010824
     WO 2001-US29432
                                20010920
OS
     MARPAT 136:279215
AB
     N-aryl- and N-heteroarylcarbonyl benzenesulfonamides I [A =
     (un) substituted Ph, 5- or 6-membered heterocyclic ring with 1-3 N, O, or S
     atoms; R1 = alkyl, haloalkyl, NO2, NR6R7; R2, R3 = H, alkyl, alkenyl,
     alkynyl, alkoxy, alkylthio, etc.; R4 = aryl, arylalkenyl, arylalkoxy,
     cycloalkenyl, cycloalkyl, halo, heterocyclyl, heterocyclyloxy; R5 = H,
     alkyl, halo; R6, R7 = H, alkenyl, alkoxyalkyl, alkoxycarbonylalkyl, alkyl,
     heterocyclyl, etc.; R6R7N = imidazolyl, morpholinyl, piperazinyl,
     piperidinyl, pyrrolidinyl, etc.] are prepared Over 500 I are prepared E.g.,
     N-biphenylcarbonyl benzenesulfonamide II was prepared by Pd-catalyzed
     coupling of 4-FC6H4B(OH)2 and 4-BrC6H4CO2Me, hydrolysis of the ester with
     LiOH, acylation of 4-chloro-3-nitrobenzenesulfonamide with the resulting
     acid in the presence of EDCI and DMAP, and nucleophilic aromatic substitution
     of the chlorobenzenesulfonamide with 2,2-dimethylcyclopentylamine.
     Compds. of the invention inhibit Bcl-Xl with IC50 values between 0.011
     \mu M and 10 \mu M , and inhibit Bcl-2 with IC50 values between 0.017 \mu M
     and 10 \muM.
```

Absolute stereochemistry.

$$\begin{array}{c|c} & & & & \\ & & & \\ \text{PhS} & & & \\ \text{H} & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\$$

RN 406230-66-8 CAPLUS
CN 3-Pyridinecarboxamide, 6-(4-fluorophenyl)-N-[[3-nitro-4-[[2-(phenylthio)ethyl]amino]phenyl]sulfonyl]- (9CI) (CA INDEX NAME)

```
ANSWER 22 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
L10
     2001:713312 CAPLUS
AN
     135:272885
DN
     Preparation of pyridinyl acylsulfimides as insecticides, acaricides, and
ΤI
     nematocides
     Kornuta, Pavel Petrovich; Shermolovich, Yuriy Grigorievich; Doeller, Uwe;
IN
     Ort, Oswald; Schaper, Wolfgang; Jans, Daniela; Sanft, Ulrich; Thoenessen,
     Maria-Theresia; Beckmann, Marion; Waibel, Jutta Maria; Pazenok, Sergiy
     Aventis CropScience GmbH, Germany; Kornuta, Nataliya Olexandrivna
PA
     PCT Int. Appl., 119 pp.
SO
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FAN.CNT 1
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     WO 2001070692
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     DE 2000-10057911
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                           Α
     WO 2001-EP3083
                                  20010317
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     US 2001-812309
                           В1
                                  20010320
OS
     MARPAT 135:272885
AB
     Title compds. [I; X = CH, N; Y = O, S; m, n = 0, 1; R1 = haloalkyl; R2, R3
     = H, halo, (O-, S-, N-interrupted) (substituted) alkyl; R4, R5 = R6, CWR7,
     C(:NOR7)R7, C(:NNR72)R7, C(:W)OR7, etc.; R6 = alkyl alkenyl, alkynyl,
     cycloalkyl, cycloalkenyl, etc.; R7 = H, R6; W = O, S; R4R5 = (substituted)
     heterocyclyl], were prepared Thus, N-(2,4,6-trimethylbenzenesulfonyl)methyl
     thien-3-ylsulfimide and 4-trifluoromethylnicotinyl chloride in CH2Cl2 were
     dropwise treated with Et3N in CH2Cl2 followed by stirring at room temperature
     for 1.5 days to give 81.6% I (R1 = CF3; R2, R3 = H; R4 = Me; R5 =
     thien-3-yl; X = CH; Y = O; m, n = 0). Tested I gave 90-100% kill of
     aphids on vicia faba.
ΙT
     362724-75-2P
     RL: AGR (Agricultural use); BAC (Biological activity or effector, except
     adverse); BSU (Biological study, unclassified); SPN (Synthetic
     preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
        (preparation of pyridinyl acylsulfimides as insecticides, acaricides, and
```

nematocides)

RN 362724-75-2 CAPLUS

CN 3-Pyridinecarboxamide, N-[N-propyl-S-(propylamino)sulfinimidoyl]-4-(tri-fluoromethyl)- (9CI) (CA INDEX NAME)

10/811,578

L10 ANSWER 23 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

AN 2001:418824 CAPLUS

DN 135:1668

TI N-heterocycloformyl-sulfonamide herbicide

IN Taisi, M. C.; Li, Bin

PA Shenyang Inst. of Chemical Engineering, Peop. Rep. China

SO Faming Zhuanli Shenqing Gongkai Shuomingshu, 12 pp. CODEN: CNXXEV

DT Patent

LA Chinese

FAN.CNT 1

~							
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE		
PI	CN 1274528	Α	20001129	CN 1999-112943	19990520		
	CN 1091349	В	20020925				
PRAI	CN 1999-112943		19990520				

OS MARPAT 135:1668

AB The herbicide I (where R = (C3-C6) alkyne or epoxy alkyl group; W = pyridine, pyrazine, pyrimidine, pyridazine, furan or thiophene; X = halo group, C1-C6 alkyl, C1-C6 haloalkyl, C1-C6 alkoxy, C1-C6 haloalkoxyl, nitro, cyano or C1-C6 alkoxycarbonyl group; and n = 0, 1, 2 or 3) is highly effective for use on maize, cotton, rice, soybean, etc.

IT 293297-28-6P 293297-30-0P 342371-46-4P
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES

(N-heterocycloformyl-sulfonamide herbicide)

RN 293297-28-6 CAPLUS

CN 3-Pyridinecarboxamide, N-[(3-chlorophenyl)sulfonyl]-N-2-propynyl-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 293297-30-0 CAPLUS

CN 3-Pyridinecarboxamide, N-[(3-methylphenyl)sulfonyl]-N-2-propynyl-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} CH_2-C \Longrightarrow CH \\ \hline 0 & 0 \\ \hline S-N-C & N \\ \hline 0 & F_3C & N \end{array}$$

RN 342371-46-4 CAPLUS

CN 3-Pyridinecarboxamide, 6-chloro-N-[(3-chlorophenyl)sulfonyl]-N-2-propynyl-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} CH_2-C \Longrightarrow CH \\ O & O \\ S-N-C & N \\ O & F_3C & C1 \\ \end{array}$$

L10 ANSWER 24 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

2001:63989 CAPLUS AN

134:131426 DN

Preparation and effect of coumarone analogues as antitumor agents TI

Fujita, Takashi; Wada, Kunio; Oguchi, Minoru; Kurakata, Shinichi IN

Sankyo Company, Ltd., Japan PA

PCT Int. Appl., 238 pp. SO

CODEN: PIXXD2

Patent DT

LA Japanese

FAN.CNT 1

os

	PATENT NO.				KIND DATE A1 20010125			APPLICATION NO. 						DATE				
ΡI	WO 2001005780			20000714														
		W:	AU, US,	•	CA,	CN,	CZ,	HU,	ID,	IL,	IN,	KR,	MX,	NO,	NZ,	PL,	RU,	TR,
		RW:	AT, PT,	•	CH,	CY,	DE,	DK,	ES,	FI,	FR,	GB,	GR,	IE,	IT,	LU,	MC,	NL,
	JP	2001	0894	68		A2		20010403 JP 2000-213985					20000714					
PRAI	JP	1999	-203	159		Α		1999	0716									

PRAI JP 1999-203159

MARPAT 134:131426

Title coumarone analogs [I; wherein R1 is hydrogen, C1-C6 alkyl; R2 is AB hydrogen, C1-C6 alkyl; R3, R5 are each independently hydrogen, C1-C6 alkyl; R4, R6 are each independently hydroxy, C1-6 alkyl, NH2, acetoxy, methoxymethoxy; X is a single bond, C=O, C=NOR7; R7 and R8 are each independently hydrogen, C1-C6 alkyl, C2-C6 alkenyl; A is C=O, SO2; U is CH2, or the like; Y is O or S; Q is hydrogen, nitro, hydroxyl; p is an integer of 1 to 6; m and n are each independently an integer of 0 to 8; and Arl and Ar2 are each benzene ring or pyridine ring] exhibiting excellent antitumor activities are prepared and formulation are discussed. Thus, title compound II was prepared and tested.

IT 321919-68-0P

> RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation and effect of coumarone analogs as antitumor agents)

RN 321919-68-0 CAPLUS

CN 3-Pyridinecarboxamide, N-[4-[[6-(acetyloxy)-3,4-dihydro-2,5,7,8tetramethyl-2H-1-benzopyran-2-yl]methoxy]-3-(trifluoromethyl)phenyl]-N-[(chloromethyl)sulfonyl]- (9CI) (CA INDEX NAME)

Me Me
$$F_3C$$
 $N-C$ N

Aco Me CH_2-O N

RE.CNT 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

```
ANSWER 25 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
L10
     2000:865121 CAPLUS
AN
     134:29435
DN
     Preparation of 2-aryl-1,2,4-triazin-3,5-di(thi)ones as herbicides.
ΤI
     Linker, Karl-Heinz; Kluth, Joachim; Drewes, Mark Wilhelm; Dahmen, Peter;
IN
     Feucht, Dieter; Pontzen, Rolf
     Bayer A.-G., Germany
PA
     Ger. Offen., 24 pp.
SO
     CODEN: GWXXBX
DT
     Patent
     German
LA
FAN.CNT 1
                          KIND
                                  DATE
                                             APPLICATION NO.
                                                                       DATE
     PATENT NO.
                          ____
     DE 19925593
                          A1
                                  20001207 DE 1999-19925593
                                                                       19990604
PΙ
     CA 2375942
                           AA
                                  20001214
                                              CA 2000-2375942
                                                                       20000524
     WO 2000075119
                           A2
                                               WO 2000-EP4704
                                                                       20000524
                                  20001214
     WO 2000075119
                          A3
                                  20010830
             AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU,
              CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL,
              IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA,
             MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM,
              AZ, BY, KG, KZ, MD, RU, TJ, TM
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
     BR 2000011330
                                  20020305
                                               BR 2000-11330
                                                                        20000524
                           Α
                                  20020327
                                               EP 2000-940265
                                                                        20000524
     EP 1189893
                           A2
     EP 1189893
                           В1
                                  20050907
         R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
              IE, SI, LT, LV, FI, RO
                                               JP 2001-501600
                                  20030114
                                                                        20000524
     JP 2003501419
                           Т2
     AU 770424
                           В2
                                  20040219
                                               AU 2000-55254
                                                                        20000524
                          E
                                               AT 2000-940265
                                                                       20000524
     AT 303999
                                  20050915
     US 2003069140
                          A1
                                  20030410
                                               US 2001-980274
                                                                       20011129
     US 6608004
                          B2
                                  20030819
PRAI DE 1999-19925593
                          Α
                                  19990604
     WO 2000-EP4704
                           W
                                  20000524
os
     MARPAT 134:29435
     Title compds. [I; Q1, Q2 = O, S; R1 = H, cyano, amino, (substituted)
     alkyl, alkoxy, alkylcarbonyl, alkoxycarbonyl, alkenyl, alkynyl,
     cycloalkyl, etc.; R2 = H, halo, NO2, CO2H, cyano, thiocarbamoyl, amino,
     (substituted) alkyl, alkoxy, alkylthio, alkenyl, alkynyl, cycloalkyl,
     etc.; R3 = H, cyano, halo; R4 = cyano, thiocarbamoyl; R5 = H,
     alkoxycarbonyl, R7, OR7, SR7, NHR7, etc.; R6 = amino, OH, R7, etc.; R7 =
     (substituted) alkyl, alkenyl, cycloalkyl, aryl, aralkyl, etc.], were
     prepared as herbicides (no data). Thus, 2-(4-cyano-2-fluoro-5-
     ethylsulfonylaminophenyl)-4-methyl-1,2,4-triazin-3,5-(2H,4H)-dione (preparation
     given), Et3N, and C1CH2CH2COCl were stirred 12 h in MeCN to give 86%
     2-[5-(N-acryloyl-N-ethylsulfonylamino)-4-cyano-2-fluorophenyl]-4-methyl-
     1,2,4-triazin-3,5-(2H,4H)-dione. The latter and other I were said to show
     very strong pre- and postemergent herbicidal activity and good crop
     tolerance.
IT
     311318-82-8P 311319-15-0P 311319-16-1P
     311319-17-2P 311319-20-7P
     RL: AGR (Agricultural use); BAC (Biological activity or effector, except
     adverse); BSU (Biological study, unclassified); SPN (Synthetic
```

preparation); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of 2-aryl-1,2,4-triazin-3,5-di(thi)ones as herbicides)

RN 311318-82-8 CAPLUS

CN 3-Pyridinecarboxamide, N-[2-cyano-5-(4,5-dihydro-4-methyl-3,5-dioxo-1,2,4-triazin-2(3H)-yl)-4-fluorophenyl]-N-(ethylsulfonyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c}
O & O & O \\
N & O & S - Et \\
N - C & O \\
N & CN & O
\end{array}$$

RN 311319-15-0 CAPLUS

CN 3-Pyridinecarboxamide, 6-chloro-N-[2-cyano-5-(4,5-dihydro-4-methyl-3,5-dioxo-1,2,4-triazin-2(3H)-yl)-4-fluorophenyl]-N-(ethylsulfonyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c}
O & O & O \\
N & O & S - Et \\
N & O & N - C \\
N & O & O
\end{array}$$
C1

RN 311319-16-1 CAPLUS

CN 3-Pyridinecarboxamide, N-[2-cyano-5-(4,5-dihydro-4-methyl-3,5-dioxo-1,2,4-triazin-2(3H)-yl)-4-fluorophenyl]-N-(ethylsulfonyl)-2-(propylthio)- (9CI) (CA INDEX NAME)

RN 311319-17-2 CAPLUS

CN 3-Pyridinecarboxamide, 5,6-dichloro-N-[2-cyano-5-(4,5-dihydro-4-methyl-3,5-dioxo-1,2,4-triazin-2(3H)-yl)-4-fluorophenyl]-N-(ethylsulfonyl)- (9CI) (CA INDEX NAME)

RN 311319-20-7 CAPLUS

CN 3-Pyridinecarboxamide, 2,6-dichloro-N-[2-cyano-5-(4,5-dihydro-4-methyl-3,5-dioxo-1,2,4-triazin-2(3H)-yl)-4-fluorophenyl]-N-(ethylsulfonyl)-5-fluoro-(9CI) (CA INDEX NAME)

10/811,578

L10 ANSWER 26 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

AN 2000:639169 CAPLUS

DN 133:233910

TI Preparation of N-(heterocyclylcarbonyl)sulfonamide herbicides

IN Tice, Colin Michael; Li, Bin

PA Rohm and Haas Company, USA

SO U.S., 6 pp.

CODEN: USXXAM

DT Patent

LA English

FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 6117821 PRAI US 1998-86263P	A P	20000912 19980521	US 1999-309432	19990511

OS MARPAT 133:233910

AB N-(heterocyclylcarbonyl)sulfonamide compds. I [W = pyridyl substituted with (C1-C6)alkyl, and optionally further substituted with 1-3 Z; R = C3-C6(alkynyl) or epoxy(C3-C6-alkyl); n = 0-3; X, Z = halo, (C1-C6)alkyl, halo(C1-C6)alkyl, (C1-C6)alkoxy, halo(C1-C6)alkoxy, nitro, cyano, or (C1-C6)alkoxycarbonyl], optionally in combination with a fertilizer, are prepared and used as broad spectrum herbicides against monocot and dicot weeds in preemergence and postemergence applications in corn, cotton, rice, soybean and wheat.

IT 293297-28-6P 293297-30-0P

RL: AGR (Agricultural use); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)

(N-(heterocyclylcarbonyl)sulfonamide herbicides)

RN 293297-28-6 CAPLUS

CN 3-Pyridinecarboxamide, N-[(3-chlorophenyl)sulfonyl]-N-2-propynyl-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 293297-30-0 CAPLUS

CN 3-Pyridinecarboxamide, N-[(3-methylphenyl)sulfonyl]-N-2-propynyl-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

10/811,578

- L10 ANSWER 27 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
- AN 2000:557420 CAPLUS
- DN 133:217856
- TI Mutational analysis of the interaction of the N- and C-terminal ends of angiotensin II with the rat AT1A receptor
- AU Costa-Neto, Claudio M.; Miyakawa, Ayumi A.; Oliveira, Laerte; Hjorth, Siv A.; Schwartz, Thue W.; Paiva, Antonio C. M.
- CS Department of Biophysics, Escola Paulista de Medicina, Federal University of Sao Paulo, Sao Paulo, 04023-062, Brazil
- SO British Journal of Pharmacology (2000), 130(6), 1263-1268 CODEN: BJPCBM; ISSN: 0007-1188
- PB Nature Publishing Group
- DT Journal
- LA English
- AB The role of different residues of the rat ATIA receptor in the interaction with the N- and C-terminal ends of angiotensin II (AngII) was studied by determining ligand binding and production of inositol phosphates (IP) in COS-7 cells

transiently expressing the following AT1A mutants: T88H, Y92H, G196I, G196W and D278E. G196W and G196I retained significant binding and IP-production properties, indicating that bulky substituents in position 196 did not affect the interaction of AngII's C-terminal carboxyl with Lys199 located three residues below. Although the T88A mutation did not affect binding, the T88H mutant had greatly decreased affinity for AngII, suggesting that substitution of Thr88 by His might hinder binding through an indirect effect. The Y92H mutation caused loss of affinity for AngII that was much less pronounced than that reported for Y92A, indicating that His in that position can fulfil part of the requirements for binding. Replacing Asp278 by Glu caused a much smaller reduction in affinity than replacing it by Ala, indicating the importance of Asp's β -carboxyl group for AngII binding. Mutations in residues Thr88, Tyr92 and Asp278 greatly reduced affinity for AngII but not for Sarl Leu8-AngII, suggesting unfavorable interactions between these residues and AngII's aspartic acid side-chain or N-terminal amino group, which might account for the proposed role of the N-terminal amino group of AngII in the agonist-induced desensitization (tachyphylaxis) of smooth muscles.

IT 160604-42-2, [125I]L 735286

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)

(mutational anal. of interaction of N- and C-terminal ends of angiotensin II with rat AT1A receptor)

- RN 160604-42-2 CAPLUS
- CN 3-Pyridinecarboxamide, N-[[4'-[(2-ethyl-4,6-dimethyl-1H-benzimidazol-1-yl)methyl][1,1'-biphenyl]-2-yl]sulfonyl]-5-(iodo-125I)- (9CI) (CA INDEX NAME)

Me N CH2
$$O = S = O$$

$$125I \qquad O = S = O$$

$$V = CH2$$

$$V =$$

RE.CNT 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

```
ANSWER 28 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
     1999:233898 CAPLUS
AN
     130:252154
DN
     Preparation of acylsulfamoylbenzoic acid amides as herbicide safeners.
ΤI
     Ziemer, Frank; Willms, Lothar; Auler, Thomas; Bieringer, Hermann;
IN
     Rosinger, Christopher
    Hoechst Schering Agrevo G.m.b.H., Germany
PA
     PCT Int. Appl., 71 pp.
SO
     CODEN: PIXXD2
DT
     Patent
     German
LΑ
FAN.CNT 1
                         KIND
                                DATE
                                            APPLICATION NO.
                                                                    DATE
     PATENT NO.
                         ____
     WO 9916744
                         A1
                                19990408
                                          WO 1998-EP6097
                                                                    19980924
PΙ
         W: AL, AM, AU, AZ, BA, BB, BG, BR, BY, CA, CN, CU, CZ, EE, GD, GE,
             HR, HU, ID, IL, IS, JP, KG, KP, KR, KZ, LC, LK, LR, LT, LV, MD,
             MG, MK, MN, MX, NO, NZ, PL, RO, RU, SG, SI, SK, SL, TJ, TM, TR,
             TT, UA, UZ, VN, YU, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
         RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES,
             FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI,
             CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
                                19990415
                                            DE 1997-19742951
                                                                    19970929
     DE 19742951
                          Α1
     CA 2305313
                          AA
                                19990408
                                            CA 1998-2305313
                                                                    19980924
     AU 9910265
                          A1
                                19990423
                                            AU 1999-10265
                                                                    19980924
     EP 1019368
                          A1
                                20000719
                                            EP 1998-952644
                                                                    19980924
                          В1
                                20030305
     EP 1019368
         R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, NL, SE
                                20000801
                                            BR 1998-12564
                                                                    19980924
     BR 9812564
                          Α
     JP 2001518461
                          Т2
                                20011016
                                            JP 2000-513830
                                                                    19980924
     AT 233730
                          Ε
                                20030315
                                            AT 1998-952644
                                                                    19980924
     RU 2205824
                          C2
                                20030610
                                            RU 2000-110730
                                                                    19980924
     ES 2194358
                          Т3
                                20031116
                                            ES 1998-952644
                                                                    19980924
     US 6251827
                          В1
                                20010626
                                            US 1998-161120
                                                                    19980925
                                19990329
                                            ZA 1998-8826
                                                                    19980928
     ZA 9808826
                          Α
PRAI DE 1997-19742951
                          Α
                                19970929
     WO 1998-EP6097
                          W
                                19980924
OS
     MARPAT 130:252154
     Plant protection agents optionally containing ≥1 pesticide and containing
AB
     ≥1 title compds. [I; X = CH, N; R1 = H, (substituted) heterocyclyl,
     hydrocarbyl; R2 = H, OH, (substituted) alkyl, alkenyl, alkynyl, alkoxy,
     alkenyloxy; R1R2 = atoms to form 3-8 membered ring; R3 = halo, cyano, NO2,
     amino, OH, CO2H, CHO, CONH2, SO2NH2, etc.; R4 = H, alkyl, alkenyl,
     alkynyl; R5 = halo, cyano, NO2, amino, OH, CO2H, CHO, CONH2, SO2NH2,
     phosphoryl, etc.; m = 0-5; n = 0-4; with provisos], are claimed (no data).
     Thus, 2-chlorobenzoic acid in THF was treated with carbonyldiimidazole
     followed by 30 min stirring at room temperature and 30 min. at reflux;
     N-propyl-4-sulfamoylbenzamide and then DBU were added and the mixture was
     refluxed 3 h to give 54% 4-(2-chlorobenzoylsulfamoyl)-N-propylbenzamide.
     221670-20-8P 221670-23-1P 221670-26-4P
IT
     221670-29-7P 221670-31-1P
     RL: AGR (Agricultural use); BAC (Biological activity or effector, except
     adverse); BSU (Biological study, unclassified); SPN (Synthetic
     preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
        (preparation of acylsulfamoylbenzoic acid amides as herbicide safeners)
RN
     221670-20-8 CAPLUS
     3-Pyridine carboxamide, 2-methoxy-N-[[4-[[(1-methylethyl)amino]carbonyl]phe
CN
```

nyl]sulfonyl]- (9CI) (CA INDEX NAME)

RN 221670-23-1 CAPLUS

CN 3-Pyridinecarboxamide, N-[[4-[(cyclopropylamino)carbonyl]phenyl]sulfonyl]-2-methoxy- (9CI) (CA INDEX NAME)

RN 221670-26-4 CAPLUS

CN 3-Pyridinecarboxamide, N-[[4-[[(1,2-dimethylpropyl)amino]carbonyl]phenyl]s ulfonyl]-2-methoxy- (9CI) (CA INDEX NAME)

RN 221670-29-7 CAPLUS

CN 3-Pyridinecarboxamide, N-[[2,4-dichloro-5-[(cyclopropylamino)carbonyl]phen yl]sulfonyl]-2-methoxy- (9CI) (CA INDEX NAME)

RN 221670-31-1 CAPLUS

CN 3-Pyridinecarboxamide, N-[[2-chloro-5-[(cyclopropylamino)carbonyl]phenyl]s ulfonyl]-2-methoxy- (9CI) (CA INDEX NAME)

RE.CNT 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

```
L10 ANSWER 29 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN AN 1997:178823 CAPLUS
```

DN 126:171487

- TI Preparation of aminopyridinecarboxylic acids and related compounds as inhibitors of the pain enhancing effects of E-type prostaglandins.
- IN Breault, Gloria Anne
- PA Zeneca Limited, UK; Breault, Gloria Anne
- SO PCT Int. Appl., 93 pp. CODEN: PIXXD2
- DT Patent
- LA English

FAN.CNT 1

	PA?	ENT I	NO.			KIN		DATE			API	PLI	CAT	ION	NO.		D	ATE	
PI	WO	9700 W:	AL, ES,	AM, FI, LV,	GB,	A1 AU, GE,	AZ, HU,	1997 BB, IS, MN,	BG, JP,	BR, KE,	B)	ſ, 3,	CA, KP,	CH, KR,	CN, KZ,	LK,	DE, LR,	LS,	EE, LT,
	IL CA AU	RW: 50203 1186 22203 96623 6996	KE, IE, 26 63 529 321	LS, IT,	LU,	MC, B	NL,	UG, PT, 2002 2001 1997 1997	SE, 0911 0430 0109 0122	BF,	BC TW IL	19 19	CF, 996- 996-	CG, 8510 1186	CI, 7057 63	CM,	GA, 1:	GN 9960 9960	612 616
	EP	8473 8473	91			A1 B1		1998 2001	0617		EP	19	996-	9209	37		1	9960	617
		R:	IE,	•	•	LV,	FI	ES,	·	·		•			-	NL,			•
	CN	1193	598			A B		1998 2003	0716					1963				9960	
		9608 1150				A T2 A E		1999 1999			BR JP	19	996- 997-	8908 5036	54		1:	9960 9960	
		3110 2111				A		2000 2002			NZ	19	996-	3110 9209	83		1	9960 9960	
		2824	52 58			ь В6		2002			SK	19	997-	1733			1	9960	
		8473 2169				T T3		2002 2002			PT	19	996-	9209	37		1	9960 9960	
		2909				B6		2002			CZ	19	997-	9209 4110	31		1	9960 9960	
		2198				C2		2003			RU	19	998-	4110 1008 9602	66		1	9960	
		9602 9605				B1 A		2002 1996			ZA	19	996-	5201			1	9960 9960	
		6100				A		2000			US	19	997-	9739	15		1	9971	
		9705 3111				A B1		1997 2001						5984				9971	219
		6377				B1		2002						1021				9980	
PRAI	GB GB WO	6313 1995 1996 1996	-124 -146 -GB1	5 443		B1 A A W		2001 1995 1996 1996	0620 0125 0617		US	20	JUU-	5413	U6		2	0000	403
os		1997 RPAT			87	A 3		1997	1216										

AB DOACHR3NR2BR1 [A = (substituted) Ph, naphthyl, pyridyl, pyrazinyl, pyridazinyl, pyrimidinyl, thienyl, thiazolyl, oxazolyl, thiadiazolyl, provided that the CH(R3)N(R2)BR1 and OD groups are positioned in a 1,2 relationship to one another on ring carbon atoms and the ring atom positioned ortho to the OD linking group (and therefore in the 3-position

relative to the CHR3NR2 linking group) is not substituted; B = (substituted) Ph, pyridyl, thiazolyl, oxazolyl, thienyl, thiadiazolyl, imidazolyl, pyrazinyl, pyridazinyl, pyrimidinyl; R1 = CO2H, carboxyalkyl, tetrazolyl, tetrazolylalkyl, tetronic acid, hydroxamic acid, sulfonic acid, aminocarbonyl, azolyl, etc., and is positioned on ring B in a 1,3 or 1,4 relationship with the CH(R3)N(R2) group; R2 = H, (substituted) alkyl, alkenyl, (provided the double bond is not in the 1-position), alkynyl (provided the triple bond is not in the 1-position), phenylalkyl, pyridylalkyl; R3 = H, Me, Et; D = H, (substituted) 5-7 membered carbocyclic ring containing 1 double bond, alkyl substituted by a (substitute) 5-7 membered carbocyclic ring containing 1 double bond, (CH2)nCH(R4)C(R5):CR6R7; R4 = H, Me, Et; R5 = H, Me, Br, C1, F, CF3; R6,R7 = H, alkyl, Br, Cl, F, CF3; n = 0, 1; and N- and S-oxides thereof, with specific exceptions], were prepared Thus, Me 2-[N-[5-bromo-2-(2chloroallyloxy)benzyl]-N-ethylamino]-5-pyridylcarboxylate (preparation given) was stirred with aqueous NaOH in MeOH to give 2-[N-[5-bromo-2-(2chloroallyloxy)benzyl]-N-ethylamino]-5-pyridylcarboxylic acid. Tested title compds. inhibited PGE2-induced contraction of guinea pig ileum with pA2 > 5.3.

IT 187229-70-5P 187229-71-6P 187229-72-7P 187229-73-8P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of aminopyridazinecarboxylic acids and related compds. as inhibitors of the pain enhancing effects of E-type prostaglandins)

RN 187229-70-5 CAPLUS

CN 3-Pyridinecarboxamide, 6-[[[5-bromo-2-[(2-methyl-2-propenyl)oxy]phenyl]methyl]ethylamino]-N-(phenylsulfonyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & & \\ & & & & \\ & & & \\ \text{Ph}-\text{S}-\text{NH}-\text{C} & & \\ \parallel & \parallel & \\ \text{O} & \text{O} & \\ \end{array}$$

RN 187229-71-6 CAPLUS

CN 3-Pyridinecarboxamide, 6-[[[5-bromo-2-[(2-methyl-2propenyl)oxy]phenyl]methyl]ethylamino]-N-(propylsulfonyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & & & \\ & &$$

RN 187229-72-7 CAPLUS

CN 3-Pyridinecarboxamide, 6-[[[5-bromo-2-[(2-chloro-2-propenyl)oxy]phenyl]methyl]ethylamino]-N-(phenylsulfonyl)- (9CI) (CAINDEX NAME)

$$\begin{array}{c|c} & & & & & \\ & & & & \\ & & & \\ Ph-S-NH-C & & & \\ & & & \\ Ph-S-NH-C & & \\ & & & \\ & & & \\ O & O & \\ \end{array}$$

RN 187229-73-8 CAPLUS

CN 3-Pyridinecarboxamide, 6-[[[5-bromo-2-[(2-chloro-2-propenyl)oxy]phenyl]methyl]ethylamino]-N-(propylsulfonyl)- (9CI) (CA INDEX NAME)

- L10 ANSWER 30 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
- AN 1996:666870 CAPLUS
- DN 125:301001
- TI Preparation of 3-(2'-sulfamoylbiphenyl-4-yl)methyl-2-imino-1,3,4-thiazolidine derivatives as antihypertensives
- IN Sakae, Shinya; Yokomoto, Masaharu; Inoe, Satoshi; Nishimura, Koji; Hirata, Akikage; Iguma, Kenichi; Tamura, Koichi
- PA Wakunaga Seiyaku Kk, Japan
- SO Jpn. Kokai Tokkyo Koho, 31 pp. CODEN: JKXXAF
- DT Patent
- LA Japanese
- FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
ΡI	JP 08208632	A2	19960813	JP 1995-280093	19951027
PRAI	JP 1995-280093	Α	19951027		
	JP 1994-264755		19941028		

- OS MARPAT 125:301001
- AB The title compds. [I; R1 = H, COR2; wherein R2 = (un)substituted lower alkyl, cycloalkyl, or cycloalkenyl, (un)substituted aryl-lower alkyl or aryl-lower alkenyl, Ph, or aromatic heterocyclyl, lower alkoxy or aralkyloxy; R3 = halo, lower alkyl or cycloalkyl, (un)substituted Ph, lower alkyl alkoxy; R4 = H, lower alkyl, acyl; R5, R6 = H, halo, lower alkyl], which show potent angiotensin II-antagonizing, smooth muscle-relaxing, and antihypertensive activity, are prepared Thus, 533 mg 5-ethyl-2-trifluoroacetamido-1,3,4-thiadiazole and 1.00 g 4-bromomethyl-2'-(N-tert-butylsulfamoylbiphenyl-4-yl)biphenyl were added to DMF and stirred at room temperature for 4 h to give 606 mg I (R1 = CF3CO, R3 = Et, R5 = R6 = H, R4 = tert-butyl). I (R1 = Q, R3 = Et, R4 = CO2Et, R5 = R6 = H) and I (R1 = 2-ClC6H4CO, R3 = Et, R4 = COC6H4CO2Me-2, R5 = R6 = H) in vitro showed IC50 of 3.0 and 5.3 nM, resp., for inhibiting angiotensin II and in vivo inhibited angiotensin II-induced hypertension of rats by 53.4 and 62.3%, resp., at 0.1 mg/kg i.v.
- IT 183000-06-8P 183000-42-2P
 - RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 - (preparation of [(sulfamoylbiphenylyl)methyl]iminothiazolidine derivs. as antihypertensives, angiotensin II antagonists, and smooth muscle relaxants)
- RN 183000-06-8 CAPLUS
- CN 3-Pyridinecarboxamide, N-[[4'-[[2-[(cyclopropylcarbonyl)imino]-5-ethyl-1,3,4-thiadiazol-3(2H)-yl]methyl][1,1'-biphenyl]-2-yl]sulfonyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & & & \\ & & & & & \\ & & & & \\ & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ &$$

RN 183000-42-2 CAPLUS

CN 3-Pyridinecarboxamide, 2-chloro-N-[[4'-[[2-[(cyclopropylcarbonyl)imino]-5-ethyl-1,3,4-thiadiazol-3(2H)-yl]methyl][1,1'-biphenyl]-2-yl]sulfonyl]-(9CI) (CA INDEX NAME)

```
L10 ANSWER 31 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
     1996:367337 CAPLUS
AN
     125:33683
DN
     Aromatic amino ethers as pain relieving agents
ΤI
     Breault, Gloria Anne; Oldfield, John; Tucker, Howard; Warner, Peter
IN
     Zeneca Limited, UK
PA
     PCT Int. Appl., 140 pp.
so
     CODEN: PIXXD2
DT
     Patent
     English
LA
FAN.CNT 1
     PATENT NO.
                         KIND
                                DATE
                                            APPLICATION NO.
                                                                   DATE
                         ____
                                            _____
                                19960208
                                           WO 1995-GB1728
                                                                   19950721
PΙ
     WO 9603380
                         A1
         W: AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI,
             GB, GE, HU, JP, KE, KG, KP, KR, KZ, LK, LR, LT, LU, LV, MD, MG,
            MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM,
            TT, UA
         RW: KE, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT,
             LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE,
             SN, TD, TG
                                            CA 1995-2192088
                                19960208
                                                                   19950721
     CA 2192088
                          AΑ
                                            AU 1995-29883
                                                                   19950721
     AU 9529883
                          A1
                                19960222
     AU 688541
                          B2
                                19980312
                                                                   19950721
     EP 773930
                         A1
                                19970521
                                            EP 1995-925943
     EP 773930
                          В1
                                20001011
         R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE
                                19970709
                                            CN 1995-194340
                                                                   19950721
     CN 1154106
                          Α
     CN 1085663
                          В
                                20020529
     BR 9508335
                         Α
                                19970930
                                            BR 1995-8335
                                                                   19950721
     HU 76606
                         A2
                                19971028
                                            HU 1996-3338
                                                                   19950721
     JP 10503487
                         T2
                                19980331
                                            JP 1995-505573
                                                                   19950721
     AT 196898
                         Ε
                                20001015
                                            AT 1995-925943
                                                                   19950721
     ES 2150577
                         Т3
                                20001201
                                            ES 1995-925943
                                                                   19950721
                         T
                                            PT 1995-925943
                                                                   19950721
     PT 773930
                                20010131
     TW 411328
                         В
                                20001111
                                            TW 1995-84107606
                                                                   19950722
     ZA 9506149
                        Α
                                19960207
                                            ZA 1995-6149
                                                                   19950724
     FI 9700261
                        Α
                                19970122
                                            FI 1997-261
                                                                   19970122
     FI 116219
                        В1
                                20051014
     NO 9700314
                        Α
                                19970313
                                            NO 1997-314
                                                                   19970124
                        B1
     NO 308032
                                20000710
     US 5843942
                        Α
                                19981201
                                            US 1997-776275
                                                                   19970124
     CN 1286254
                        Α
                                20010307
                                            CN 2000-104017
                                                                   20000310
     GR 3034603
                         Т3
                                20010131
                                            GR 2000-402119
                                                                   20001012
PRAI GB 1994-14924
                         Α
                                19940725
     GB 1995-1288
                         A
                                19950124
     WO 1995-GB1728
                          W
                                19950721
os
     MARPAT 125:33683
     The invention relates to compds. I [A = (un)substituted Ph, naphthyl,
AΒ
     pyridyl, pyrazinyl, pyridazinyl, pyrimidyl, thienyl, thiazolyl, oxazolyl,
     thiadiazolyl having ≥ 2 adjacent ring C atoms, or bicyclic ring
     system, provided that the shown sidechains on A are in a 1,2-relationship,
     and the 3-position is unsubstituted; B, D = (un)substituted ring system;
     R1 = various groups; R2 = H, alk(en/yn)yl, phenylalkyl, 5- or 6-membered
     heteroarylalkyl; R3, R4 = H or alkyl] and their N-oxides, S-oxides,
     pharmaceutically acceptable salts, and in vivo-hydrolyzable esters and
     amides. Also claimed are processes for their preparation, intermediates, use
     as therapeutic agents, and pharmaceutical compns. I are analgesics which
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are structurally different from NSAIDS and opiates, and which may also possess antiinflammatory, antipyretic, and antidiarrheal properties. For example, condensation of 6-chloropyridazine-3-carboxamide with N-ethyl-N-(2-benzyloxy-5-bromobenzyl)amine-HCl in N-methylpyrrolidinone containing NaHCO3 at 115 $^{\circ}$ (85 $^{\circ}$), and hydrolysis of the carboxamide function with NaOH in iso-PrOH (97 $^{\circ}$), gave title compound II. I generally had pA2 > 5.3 for inhibition of PGE2-induced contraction of guinea pig ileum in vitro, and ED50 of 0.01-100 mg/kg orally in the i.p.-induced writhing test.

177758-29-1P 177758-44-0P 177758-45-1P 177758-46-2P 177758-47-3P 177758-48-4P 177758-49-5P 177758-50-8P 177758-51-9P 177758-52-0P 177758-53-1P 177758-56-4P 177758-98-4P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of aromatic amino ethers as analgesics)

RN 177758-29-1 CAPLUS

CN 3-Pyridinecarboxamide, 6-[[[5-bromo-2-(phenylmethoxy)phenyl]methyl]ethylam ino]-N-(phenylsulfonyl)- (9CI) (CA INDEX NAME)

RN 177758-44-0 CAPLUS

CN 3-Pyridinecarboxamide, 6-[[[5-bromo-2-(phenylmethoxy)phenyl]methyl]ethylam ino]-N-(propylsulfonyl)- (9CI) (CA INDEX NAME)

RN 177758-45-1 CAPLUS

CN 3-Pyridinecarboxamide, N-[[5-(acetylamino)-1,3,4-thiadiazol-2-yl]sulfonyl]-6-[[[5-bromo-2-(phenylmethoxy)phenyl]methyl]ethylamino]- (9CI) (CA INDEX NAME)

RN 177758-46-2 CAPLUS

CN 3-Pyridinecarboxamide, 6-[[[5-bromo-2-(phenylmethoxy)phenyl]methyl]ethylam ino]-N-[[5-(2-pyridinyl)-2-thienyl]sulfonyl]- (9CI) (CA INDEX NAME)

RN 177758-47-3 CAPLUS

CN 3-Pyridinecarboxamide, 6-[[[5-bromo-2-(phenylmethoxy)phenyl]methyl]ethylam ino]-N-[(3,5-dimethyl-4-isoxazolyl)sulfonyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

RN 177758-48-4 CAPLUS

CN 3-Pyridinecarboxamide, 6-[[[5-bromo-2-(phenylmethoxy)phenyl]methyl]ethylam ino]-N-[(2-hydroxyethyl)sulfonyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \mathsf{Br} \\ \mathsf{HO-CH_2-CH_2-S-NH-C} \\ \mathsf{O} \\ \\ \mathsf{O} \\ \\ \mathsf{Ph-CH_2-O} \\ \end{array}$$

RN 177758-49-5 CAPLUS

CN 3-Pyridinecarboxamide, 6-[ethyl[[5-(methylsulfonyl)-2-(phenylmethoxy)phenyl]methyl]amino]-N-[(phenylmethyl)sulfonyl]- (9CI) (CA INDEX NAME)

RN 177758-50-8 CAPLUS

CN 3-Pyridinecarboxamide, 6-[[[5-bromo-2-(phenylmethoxy)phenyl]methyl]ethylam ino]-N-[(1,3,5-trimethyl-1H-pyrazol-4-yl)sulfonyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

RN 177758-51-9 CAPLUS

CN 3-Pyridinecarboxamide, 6-[[[5-bromo-2-(phenylmethoxy)phenyl]methyl]ethylam ino]-N-[(5-chloro-2-thienyl)sulfonyl]- (9CI) (CA INDEX NAME)

C1
$$S = NH - C = N$$
 Et $O - CH_2 - Ph$ $O - CH_2 - Ph$

RN 177758-52-0 CAPLUS

CN 3-Pyridinecarboxamide, 6-[[[5-bromo-2-(phenylmethoxy)phenyl]methyl]ethylam

ino]-N-[(4-fluorophenyl)sulfonyl]- (9CI) (CA INDEX NAME)

RN 177758-53-1 CAPLUS

CN 3-Pyridinecarboxamide, 6-[[[5-bromo-2-(phenylmethoxy)phenyl]methyl]ethylam ino]-N-[(tetrahydro-1,1-dioxido-3-thienyl)sulfonyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

RN 177758-56-4 CAPLUS

CN 3-Pyridinecarboxamide, 6-[ethyl[[2-(phenylmethoxy)phenyl]methyl]amino]-N-[(2-hydroxyethyl)sulfonyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & & & \\ \text{HO-CH}_2\text{-CH}_2\text{-} & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ & &$$

RN 177758-98-4 CAPLUS

CN 3-Pyridinecarboxamide, 6-[[[5-bromo-2-(phenylmethoxy)phenyl]methyl]ethylam ino]-N-[[5-[(methylamino)carbonyl]-1,3,4-thiadiazol-2-yl]sulfonyl]- (9CI) (CA INDEX NAME)

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L10 ANSWER 32 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
     1995:995215 CAPLUS
AN
     124:117098
DN
     Preparation of pyridylanilide derivatives as fungicides
TI
     Riordan, Peter Dominic; Boddy, Ian Kenneth; Osbourn, Susan Elisabeth
IN
     Agrevo UK Ltd., UK
PA
     PCT Int. Appl., 35 pp.
SO
     CODEN: PIXXD2
DT
     Patent
LΑ
     English
FAN.CNT 1
                       KIND
                                DATE
                                           APPLICATION NO.
                                                                   DATE
     PATENT NO.
                                19950928 WO 1995-GB570
ΡI
     WO 9525723
                         A1
         W: AU, BG, BR, CA, CN, CZ, FI, HU, JP, KR, KZ, MX, NO, NZ, PL, RO,
             RU, SD, SK, UA, US
         RW: KE, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT,
             LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE,
             SN, TD, TG
                                                                   19950316
                                19951009
                                            AU 1995-18981
     AU 9518981
                          Α1
     AU 688473
                          B2
                                19980312
     EP 750611
                                            EP 1995-911403
                                                                   19950316
                          A1
                                19970102
     EP 750611
                         В1
                                19980708
         R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE
     CN 1143954
                         Α
                                19970226
                                            CN 1995-192131
                                                                   19950316
     HU 74778
                                            HU 1996-2547
                                                                   19950316
                         A2
                                19970228
     HU 214292
                         В
                                19980302
                      A
T2
                                            BR 1995-7105
                                                                   19950316
     BR 9507105
                                19970909
     JP 09510471
                                19971021
                                            JP 1995-524455
                                                                   19950316
                        E
     AT 168099
                                19980715
                                            AT 1995-911403
                                                                   19950316
     ZA 9502205
                        Α
                                19951031
                                            ZA 1995-2205
                                                                   19950317
     US 5756524
                        Α
                                19980526
                                            US 1996-714149
                                                                   19960918
                        Α
                                19940318
PRAI GB 1994-5347
                                19950316
     WO 1995-GB570
                         W
     MARPAT 124:117098
OS
     Title compds. I [X = O, S; R1, R2 = H, alkyl, cycloalkyl, alkenyl, etc.;
AB
     R3 = (substituted) pyridyl, pyrimidinyl, pyrazinyl, etc.] were prepared
     Condensation of 6-methoxynicotinoyl chloride with Me anthranilate in the
     presence of Et3N in THF afforded I (X = 0; R1 = R2 = H; R3 =
     6-methoxy-3-pyridyl) which showed activity against barley powdery mildew,
     rice blast and apple scab at \leq 500 ppm.
IT
     173056-79-6P
     RL: AGR (Agricultural use); BAC (Biological activity or effector, except
     adverse); BSU (Biological study, unclassified); SPN (Synthetic
     preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
        (preparation of anilide derivs. as fungicides)
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Benzoic acid, 2-[[(6-methoxy-3-pyridinyl)carbonyl](methylsulfonyl)amino]-,

RN

CN

173056-79-6 CAPLUS

methyl ester (9CI) (CA INDEX NAME)

- L10 ANSWER 33 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
- AN 1995:607987 CAPLUS
- DN 123:286034
- TI Substituted triazolinones, triazolinethiones, and triazolinimines as angiotensin II antagonists
- IN Ashton, Wallace T.; Chang, Linda L.; MacCoss, Malcolm; Chakravarty, Prasun K.; Greenlee, William J.; Patchett, Arthur A.; Flanagan, Kelly
- PA Merck and Co., Inc., USA
- SO U.S., 90 pp. Cont.-in-part of U.S. Ser. No. 899,868, abandoned. CODEN: USXXAM
- DT Patent
- LA English
- FAN.CNT 3

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
		-			
ΡI	US 5411980	Α	19950502	US 1992-994228	19921221
	ZA 9204916	Α	19930331	ZA 1992-4916	19920702
PRAI	US 1989-386328	B2	19890728		
	US 1990-504507	B2	19900404		
	US 1991-725720	B2	19910703		
	US 1991-812891	B2	19911220		
	US 1992-899868	B2	19921217		
~ ~	MADDAM 100.00/004				

- OS MARPAT 123:286034
- AB There are disclosed new substituted triazolinone compds. I [R2a = H, halo; R2b = H, halo, C1-4-alkyl; R3a = H, halo; R3b = H, halo, C1-4-alkyl; E is a single bond; R6 = (un)substituted C1-6-alkyl; R23 = e.g., (un) substituted Ph, branched C3-7-alkyl, C3-7-cycloalkyl; V1 = H, Me, CF3, halogen, with the proviso that V1 = CF3 when V2 = H; V2 = e.g., H, NO2, NR10R21; R10 = H, C1-4-alkyl; R21 = H or R22; R22 = e.g., C1-6-alkyl, C3-7-cycloalkyl; aryl] which are useful as angiotensin II antagonists. Thus, e.g., reaction of 4-bromomethyl-2'-(t-butoxycarbonyl)biphenyl with K phthalimide afforded 82% N-[[2'-(t-butoxycarbonyl)biphenyl-4yl]methyl]phthalimide; hydrazinolysis afforded 88% 4-aminomethyl-2'-(tbutoxycarbonyl)biphenyl; reaction with CS2/MeI afforded 84% Me N-[[2'-(t-butoxycarbonyl)biphenyl-4-yl]methyl]dithiocarbamate; reaction of the latter with hydrazine afforded 79% 4-[[2'-(t-butoxycarbonyl)biphenyl-4yl]methyl]-3-thiosemicarbazide; heterocyclization with tri-Me orthovalerate afforded 63% 4-[[2'-(t-butoxycarbonyl)biphenyl-4-yl]methyl]-5-butyl-2,4-dihydro-3H-1,2,4-triazole-3-thione; removal of the t-Bu group with trifluoroacetic acid afforded the corresponding 2'-carboxy derivative (21%). Representative compds. of the invention act as angiotensin II receptor antagonists with activity of at least IC50 < 50 μ M. Pharmaceutical formulations were given.
- IT 159044-96-9P
 - RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 - (substituted triazolinones, triazolinethiones, and triazolinimines as angiotensin II antagonists)
- RN 159044-96-9 CAPLUS
- CN 3-Pyridinecarboxamide, N-[[4'-[[3-butyl-1,5-dihydro-5-oxo-1-[2-(trifluoromethyl)phenyl]-4H-1,2,4-triazol-4-yl]methyl][1,1'-biphenyl]-2-yl]sulfonyl]-2-chloro-(9CI) (CA INDEX NAME)

- L10 ANSWER 34 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
- AN 1995:354646 CAPLUS
- DN 123:83393
- TI Pyridine derivatives, herbicidal composition containing them, and method for killing weeds
- IN Miyazaki, Masahiro; Matsuzawa, Masafumi; Toriyabe, Keiji; Hirata, Michiya
- PA Kumiai Chemical Industries Co., Ltd., Japan; Ihara Chemical Industries Co., Ltd.
- SO U.S., 45 pp. Cont.-in-part of U.S. Ser. No. 927,281. CODEN: USXXAM
- DT Patent
- LA English
- FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 5380700	Α	19950110	US 1992-996042	19921223
	JP 05331163	A2	19931214	JP 1991-84556	19910326
	US 5385880	Α	19950131	US 1992-927281	19920917
	IN 178208	Α	19970315	IN 1994-CA798	19940930
	IN 178419	Α	19970419	IN 1994-CA799	19940930
PRAI	JP 1991-84556	Α	19910326		
	US 1992-927281	A2	19920917		
	WO 1992-JP362	W	19920326		
	IN 1992-CA401	A1	19920604		
	IN 1992-CA402	A1	19920604		

OS MARPAT 123:83393

AB The present invention provides a novel pyridine derivative having the following general formula and its salt: I wherein R is a hydrogen atom, a hydroxyl group, an alkoxy group, an alkoxy group, and derivs.; R1 and R2 may be the same or different, and are a hydrogen atom, an alkoxy group, a halogen atom, an alkylamino group, a dialkylamino group; Z is a methine group or a nitrogen atom; X1 is an acylamino group, a cycloalkyl group, a halogen-substituted alkoxy group, an alkenyloxy group, an alkynyloxy group, an alkoxycarbonyl group, an alkylamino group, a dialkylamino group, a Ph group. The pyridine derivative and its salt of the present invention achieve an excellent herbicidal effect on annual and perennial weeds growing in paddy fields and upland fields at a very small dosage. The pyridine derivative and its salt of the present invention are safe to rice, wheat, cotton and corn, and can be suitably applied as a herbicide to a field where these plants are cultivated.

IT 147078-07-7P

RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses) (herbicidal (pyrmidinylthio) - and (triazinylthio)pyridine derivs.)

RN 147078-07-7 CAPLUS

CN 3-Pyridinecarboxamide, 4-(3-chlorophenyl)-2-[(4,6-dimethoxy-2-pyrimidinyl)thio]-N-(methylsulfonyl)- (9CI) (CA INDEX NAME)

10/811,578

L10 ANSWER 35 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1995:316923 CAPLUS

DN 122:97140

TI Characterization of the binding of [1251]L-735,286: a new nonpeptide angiotensin II AT1 receptor radioligand

AU Chen, T. B.; Brenner, N. J.; Gibson, R. E.; Burns, H. D.; Chang, R. S. L.

CS Dep. New Lead Pharm., Pharm. Merck Res. Labs., West Point, PA, 19486, USA

SO Life Sciences (1995), 56(8), 629-35 CODEN: LIFSAK; ISSN: 0024-3205

PB Elsevier

DT Journal

LA English

AB [1251]L-735,286, a new potent and AT1-selective nonpeptide angiotensin II receptor radioligand, bound saturably to whole adrenal membranes. Scatchard and Hill plot anal. indicates a single class of high affinity (Kd = 0.5 nM) binding sites. The potencies of various angiotensin II agonists and antagonists in displacing specific [1251]L-735,286 binding are in good agreement with their potencies in displacing the binding of [1251]Sar1,Ile8-AII to adrenal AT1 receptors. The AT2 selective ligand, PD121981 had no effect on specific [1251]L-735,286 binding. In autoradiog. studies using rat kidney slices, specific labeling of [1251]L-735,286 was abolished by coincubation with saralasin. Collectively, the data indicated that [1251]L-735,286 represents a new, potent nonpeptide antagonist radioligand suitable for the study of angiotensin II AT1 receptors.

IT 160632-48-4, L 735286

RL: ARG (Analytical reagent use); BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); ANST (Analytical study); BIOL (Biological study); PROC (Process); USES (Uses)

(L-735,286 as angiotensin AT1 receptor radioligand)

RN 160632-48-4 CAPLUS

CN 3-Pyridinecarboxamide, N-[[4'-[(2-ethyl-4,6-dimethyl-1H-benzimidazol-1-yl)methyl][1,1'-biphenyl]-2-yl]sulfonyl]- (9CI) (CA INDEX NAME)

Me N Et
$$O = S = O$$
 $O = N + CH_2$ $O = S = O$ $O = N + CH_2$ $O = S = O$

IT 160604-42-2, [125I]L 735286

RL: ARG (Analytical reagent use); BPR (Biological process); BSU (Biological study, unclassified); ANST (Analytical study); BIOL (Biological study); PROC (Process); USES (Uses)

(L-735,286 as angiotensin AT1 receptor radioligand)

RN 160604-42-2 CAPLUS

CN 3-Pyridinecarboxamide, N-[[4'-[(2-ethyl-4,6-dimethyl-1H-benzimidazol-1-yl)methyl][1,1'-biphenyl]-2-yl]sulfonyl]-5-(iodo-125I)- (9CI) (CA INDEX NAME)

Me N
$$CH_2$$
 $O = S = O$

$$125I$$

$$N CH_2$$

$$O = S = O$$

$$N CH_2$$

- L10 ANSWER 36 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
- AN 1994:700817 CAPLUS
- DN 121:300817
- TI Triazolinone Biphenylsulfonamide Derivatives as Orally Active Angiotensin II Antagonists with Potent AT1 Receptor Affinity and Enhanced AT2 Affinity
- AU Ashton, Wallace T,; Chang, Linda L.; Flanagan, Kelly L.; Hutchins, Steven M.; Naylor, Elizabeth M.; Chakravarty, Prasun K.; Patchett, Arthur A.; Greenlee, William J.; Chen, Tsing-Bau; Faust, Kristie A.; Chang, Raymond S. L.; Lotti, Victor J.; Zingaro, Gloria J.; Schorn, Terry W.; Siegl, Peter K. S.; Kivlighn, Salah D.
- CS Merck Research Laboratories, Rahway, NJ, 07065, USA
- SO Journal of Medicinal Chemistry (1994), 37(17), 2808-24 CODEN: JMCMAR; ISSN: 0022-2623
- DT Journal
- LA English
- Several series of 2,4-dihydro-2,4,5-trisubstituted-3H-1,2,4-triazol-3-ones AΒ with acidic sulfonamide replacements of tetrazole at the 2'-position of the biphenyl-4-ylmethyl side chain at N4 were prepared and tested as angiotensin II (AII) antagonists. Preferred substituents on the triazolinone ring were Bu at C5 and 2-(trifluoromethyl)phenyl at N2. Subnanomolar IC50 values at the AT1 receptor subtype were observed for a variety of acylsulfonamides, including aroyl, heteroaroyl, and cycloalkylcarbonyl derivs. Certain other acidic sulfonamides, such as sulfonylcarbamates and disulfimides also displayed high affinity for the AT1 receptor. In addition, AT2 binding for some of these compds. was increased by as much as 1000-fold over the corresponding tetrazole, e.g. AT2 IC50 17 nM for I (R = Me3CO). When evaluated for inhibition of the AII pressor response, the benchmark benzoylsulfonamide I (R = Ph) (L-159,913) was efficacious in several species and was superior to losartan in conscious rhesus monkeys. Several subsequent analogs, including the I (R = 2-ClC6H4, 3-chlorothiophene-2-yl, (S)-2,2-dimethylcyclopropyl, Me3CO) derivs., were highly effective in rats, surpassing I (R = Ph) and losartan in duration of action and/or potency. Compound I (R = 2-ClC6H4) (L-162,223) displayed very prolonged AII antagonism in the rat model (>24 h at 1 mg/kg i.v.). At 1 mg/kg po in rats, I (R = 2-C1C6H4) and I (R = Me3C0) (L-162,234) produced 85-87% peak inhibition of the AII pressor response with duration exceeding 6 h. The identification of triazolinone-based sulfonamide derivs. combining high AT1 affinity, considerably enhanced AT2 potency, and favorable in vivo properties provides insights relevant to the design of dual AT1/AT2 receptor antagonists.
- IT 159044-96-9P
 - RL: SPN (Synthetic preparation); PREP (Preparation) (preparation and angiotensin II antagonist activity of)
- RN 159044-96-9 CAPLUS
- CN 3-Pyridinecarboxamide, N-[[4'-[[3-butyl-1,5-dihydro-5-oxo-1-[2-(trifluoromethyl)phenyl]-4H-1,2,4-triazol-4-yl]methyl][1,1'-biphenyl]-2-yl]sulfonyl]-2-chloro-(9CI) (CA INDEX NAME)

10/811,578

- L10 ANSWER 37 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
- AN 1994:605212 CAPLUS
- DN 121:205212
- TI Preparation of nicotinamides as pesticides
- IN Toki, Tadaaki; Koyanagi, Toru; Morita, Masayuki; Yoneda, Tetsuo; Kagimoto, Chiharu; Okada, Hiroshi
- PA Ishihara Sangyo Kaisha, Ltd., Japan
- SO Eur. Pat. Appl., 39 pp. CODEN: EPXXDW
- DT Patent
- LA English
- FAN. CNT 1

FAN.	CNT 1				DATE VIN
	PATENT NO.		DATE	APPLICATION NO.	DATE J
PI	EP 580374 EP 580374	A1	19940126 19960103	EP 1993-305622	19930716
					MC NI DE CE
				B, GR, IE, IT, LI, LU,	
	JP 06321903			JP 1993-214766	13330630
	JP 2994182		19991227	CD 1002 2100011	19930707
	CA 2100011			CA 1993-2100011	19930707
	CA 2100011	C	19980203	ED 1002 E042	10020712
	ZA 9305042	A		ZA 1993-5042	19930713
	IL 106340			IL 1993-106340 SK 1993-750	
		В6			19930715
		E	19960115		
	ES 2085118	Т3		ES 1993-305622	
		A1		AU 1993-42106	19930721
	AU 657056		19950223	1000 0060	10000700
	BR 9302960	A		BR 1993-2960	
	RU 2083562			RU 1993-50289	
		B1		PL 1993-299769	
	CN 1081670	Α	19940209	CN 1993-109092	19930723
	CN 1044233	В	19990721		
	US 5360806	Α		us 1993-95192	19930723
	HU 68334			HU 1993-2144	19930723
	HU 214279	В	19980302		
	CZ 286147			CZ 1993-1502	19930723
PRAI	JP 1992-238804	A	19920723		
	JP 1993-57668		19930205		
	JP 1993-96428	Α	19930317		

OS MARPAT 121:205212

AB Title compds. [I; R = halomethyl; R1,R2 = H, (cyclo)alkyl, alkenyl, alkysulfonyl, etc.; NR1R2 = heterocyclyl; X = O or S; m = 0 or 1] were prepared Thus, 4-trifluoromethylpyridine-3-carboxylic acid was amidated by H2NCH2CN to give title compound II which gave complete control of Myzus persicae larvae on eggplant leaf dipped in an 800ppm solution

IT 158063-11-7P 158063-57-1P 158063-60-6P
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of, as pesticide)

RN 158063-11-7 CAPLUS

CN 3-Pyridinecarboxamide, N-(cyanomethyl)-N-(methylsulfonyl)-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c}
 & O \\
 & | \\
 & | \\
 & S - Me \\
 & C - N - CH_2 - CN \\
 & | \\
 & CF_3 & O
\end{array}$$

RN 158063-57-1 CAPLUS

CN 3-Pyridinecarboxamide, N-(methylsulfonyl)-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 158063-60-6 CAPLUS

CN 3-Pyridinecarboxamide, N-[(dimethylamino)sulfonyl]-4-(trifluoromethyl)-(9CI) (CA INDEX NAME)

L10 ANSWER 38 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1994:557652 CAPLUS

DN 121:157652

TI [[(Tetrazolylbiphenylyl)methyl]amino]pyridinecarboxylates as Angiotensin II Receptor Antagonists

IN Winn, Martin; De, Biswanath; Zydowsky, Thomas M.; Kerkman, Daniel J.; Debernardis, John F.; Rosenberg, Saul H.; Shiosaki, Kazumi; Basha, Fatima Z.; Tasker, Andrew S.; et al.

PA Abbott laboratories, USA

SO U.S., 98 pp. Cont.-in-part of U.S. Ser. No. 744,241. CODEN: USXXAM

DT Patent

LA English

FAN.CNT 4

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI 1	US 5250548	Α	19931005	US 1992-844351	19920302
(CA 2050723	AA	19920311	CA 1991-2050723	19910905
1	AU 9183744	A1	19920312	AU 1991-83744	19910909
	AU 647174	B2	19940317		
•	JP 04261156	A2	19920917	JP 1991-258343	19910910
i	JP 07053551	A2	19950228	JP 1993-187412	19930630
PRAI	US 1990-580400	B2	19900910		
1	us 1991-744241	A2	19910815		

OS MARPAT 121:157652

AB The title compds., [[(tetrazolylbiphenylyl)methyl]amino]pyridinecarboxylat es I (R3 = H, alkyl, halo; R5 = alkyl) were disclosed. Pharmacol. test data for I as angiotensin receptor antagonists were reported.

IT 151323-15-8P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of, as angiotensin antagonist)

RN 151323-15-8 CAPLUS

CN 3-Pyridinecarboxamide, N-(phenylsulfonyl)-2-[propyl[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]amino]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & O \\ \parallel & \parallel \\ Ph-S-NH-C \\ \parallel & & \\ O & & \\ \hline N & \\ \end{array}$$

IT 157362-03-3P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of, as intermediate for [[(tetrazolylbiphenylyl)methyl]amino]py

rimidinecarboxylate)
157362-03-3 CAPLUS

RN

3-Pyridinecarboxamide, N-(phenylsulfonyl)-2-[propyl[[2'-[1-(triphenylmethyl)-1H-tetrazol-5-yl][1,1'-biphenyl]-4-yl]methyl]amino]-CN (9CI) (CA INDEX NAME)

10/811,578

L10 ANSWER 39 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

1994:457525 CAPLUS AN

121:57525 DN

Preparation of pyrimidine derivatives as herbicides ΤI

Myazaki, Masahiro; Matsuzawa, Masafumi; Toyabe, Keiji; Hirata, Micha IN

PA Kumiai Chemical Industry Co, Japan; Ihara Chemical Ind Co

Jpn. Kokai Tokkyo Koho, 79 pp. SO

CODEN: JKXXAF

DΤ Patent

Japanese LA

FAN.CNT 1

27811	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE	
ΡI	JP 06041116	 A2	19940215	JP 1992-97313	19920325	
	JP 3217848	B2	20011015			
PRAT	JP 1992-97313		19920325			

MARPAT 121:57525 os

The title compds. [I; R = OH, alkoxy, benzyloxy, etc.; R1, R2 = alkoxy, AB alkyl, halo, etc.; X = alkyl, alkoxy, (un) substituted Ph, etc.; W = O, S, etc.; ; Z = methine, N; n = 0 - 3] are prepared A mixture of hydroxynicotinic acid ester II, K2CO3, and chloropyrimidine III in DMF was heated at 100° for 4 h to give pyrimidine IV. IV at 10 g/area gave 70-90% control of Echinochloa oryzicola.

IT 147078-07-7P

> RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of, as herbicide)

RN 147078-07-7 CAPLUS

3-Pyridinecarboxamide, 4-(3-chlorophenyl)-2-[(4,6-dimethoxy-2-CN pyrimidinyl)thio]-N-(methylsulfonyl)- (9CI) (CA INDEX NAME)

L10 ANSWER 40 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1994:270116 CAPLUS

DN 120:270116

TI Preparation of 4- or 5-(sulf)imido- and -(sulfon)amidopyridines and their N-oxides as fibrosuppressive agents

IN Weidmann, Klaus; Bickel, Martin; Guenzler-Pukall, Volkmar

PA Hoechst A.-G., Germany

SO Eur. Pat. Appl., 73 pp. CODEN: EPXXDW

DT Patent

LA German

FAN.CNT 1

t VIV.	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE			
PI	EP 567997	A1	19931103	EP 1993-106797	19930427			
	R: AT, BE, CH,	DE, DK	, ES, FR, GE	B, GR, IE, IT, LI, LU,	MC, NL, PT, SE			
	ZA 9302983	Α	19931115	ZA 1993-2983	19930428			
	CA 2095206	AA	19931031	CA 1993-2095206	19930429			
	NO 9301560	Α	19931101	NO 1993-1560	19930429			
	AU 9338225	A1	19931104	AU 1993-38225	19930429			
	CN 1079466	Α	19931215	CN 1993-105255	19930429			
	JP 06087831	A2	19940329	JP 1993-128332	19930430			
PRAI	DE 1992-4214465	Α	19920430					
	DE 1992-4224440	Α	19920724					
os	MARPAT 120:270116							
AB	Title compds. [I; 1	of A, B	= R3 and th	ne other = $XNR6R7$; $R1-$	R3 = H, alkyl,			
	alkoxy, halo, etc.;	R4 = a	group physi	.ol. convertable to a	carboxylate			
	function; R4 ≠ ester or amide; R6 = H, alkyl, protective group,							

IT 153685-23-5P 153685-24-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

Thus, Me 5-aminopyridine-2-carboxylate was amidated by 4-FC6H4SO2Cl and

(preparation and reaction of, in preparation of fibrosuppressive agent)

etc.; R7 = YR8; R8 = H, cycloalk(en)yl, (hetero)aryl, etc.; X = bond, CO; Y = SO2, CO, etc.; n = 0 or 1] were prepared as fibrosuppressives (no data).

RN 153685-23-5 CAPLUS

CN 3-Pyridinecarboxamide, 6-(hydroxymethyl)-N-[[4-[[(2-phenylethyl)amino]carbonyl]phenyl]sulfonyl]- (9CI) (CA INDEX NAME)

the product treated with LAH to give title compd, II.

RN 153685-24-6 CAPLUS

CN 3-Pyridinecarboxamide, N-[[4-[2-[(2-chloro-5-methoxybenzoyl)amino]ethyl]ph enyl]sulfonyl]-6-(chloromethyl)-, monosodium salt (9CI) (CA INDEX NAME)

Na

RN 153685-03-1 CAPLUS
CN 3-Pyridinecarboxamide, 6-(ethoxymethyl)-N-(phenylsulfonyl)- (9CI) (CF INDEX NAME)

RN 153685-04-2 CAPLUS

CN 3-Pyridinecarboxamide, N-[(4-butoxyphenyl)sulfonyl]-6-(methoxymethyl)-(9CI) (CA INDEX NAME)

RN 153685-05-3 CAPLUS

CN 3-Pyridinecarboxamide, N-[(4-butoxyphenyl)sulfonyl]-6-(hydroxymethyl)-(9CI) (CA INDEX NAME)

RN 153685-06-4 CAPLUS

CN 3-Pyridinecarboxamide, 6-(hydroxymethyl)-N-[[4-[[(2-phenylethyl)amino]carbonyl]phenyl]sulfonyl]-, monoammonium salt (9CI) (CA INDEX NAME)

NH3

RN 153685-07-5 CAPLUS

CN 3-Pyridinecarboxamide, N-[[4-[2-[(2-chloro-5-methoxybenzoyl)amino]ethyl]ph enyl]sulfonyl]-6-(hydroxymethyl)-, monosodium salt (9CI) (CA INDEX NAME)

Na

RN 153685-08-6 CAPLUS

CN 3-Pyridinecarboxamide, N-[[4-[(butylamino)carbonyl]phenyl]sulfonyl]-6-[(phenylmethoxy)methyl]- (9CI) (CA INDEX NAME)

RN 153685-09-7 CAPLUS

CN 3-Pyridinecarboxamide, N-[[4-[2-[(2-methyl-1-oxopropyl)amino]ethyl]phenyl] sulfonyl]-6-[(phenylmethoxy)methyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c} O \\ \text{i-Pr-C-NH-CH}_2\text{-CH}_2\text{-CH}_2\\ \\ \text{O} \\ \text{O$$

RN 153685-10-0 CAPLUS

CN 3-Pyridinecarboxamide, N-[[4-[2-[(4-methyl-1-oxopentyl)amino]ethyl]phenyl] sulfonyl]-6-[(phenylmethoxy)methyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 1-B

-- CH₂-- Ph

RN 153685-11-1 CAPLUS

CN 3-Pyridinecarboxamide, N-[[4-[[(2-phenylethyl)amino]carbonyl]phenyl]sulfon yl]-6-[(phenylmethoxy)methyl]- (9CI) (CA INDEX NAME)

RN 153685-12-2 CAPLUS

CN 3-Pyridinecarboxamide, 6-(ethoxymethyl)-N-[[4-[[(2-phenylethyl)amino]carbonyl]phenyl]sulfonyl]- (9CI) (CA INDEX NAME)

RN 153685-13-3 CAPLUS

CN 3-Pyridinecarboxamide, N-[[4-[2-[(cyclohexylacetyl)amino]ethyl]phenyl]sulf onyl]-6-(ethoxymethyl)- (9CI) (CA INDEX NAME)

RN 153685-14-4 CAPLUS

CN 3-Pyridinecarboxamide, 6-(ethoxymethyl)-N-[[4-[2-[(1-oxohexyl)amino]ethyl]phenyl]sulfonyl]- (9CI) (CA INDEX NAME)

RN 153685-15-5 CAPLUS

CN 3-Pyridinecarboxamide, 6-(ethoxymethyl)-N-[[4-[2-[(4-methyl-1-oxopentyl)amino]ethyl]phenyl]sulfonyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c} O \\ \parallel \\ Me_2CH-CH_2-CH_2-C-NH-CH_2-CH_2 \\ \hline \\ O \\ \hline \\ S-NH-C \\ \hline \\ O \\ \end{array}$$

RN 153685-16-6 CAPLUS

CN 3-Pyridinecarboxamide, N-[[4-[(butylamino)carbonyl]phenyl]sulfonyl]-6-(ethoxymethyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{n-BuNH-C} & \text{O} & \text{O} & \text{N} & \text{CH}_2\text{-OEt} \\ & \text{S-NH-C} & \text{N} & \text{CH}_2\text{-OEt} \\ & \text{O} & \text{O} & \text{O} & \text{O} \\ & \text{O} & \text{O} & \text{O} & \text{O} \\ & \text{O} & \text{O} & \text{O} & \text{O} \\ & \text{O} & \text{O} & \text{O} & \text{O} \\ & \text{O} & \text{O} & \text{O} & \text{O} \\ & \text{O} & \text{O} & \text{O} & \text{O} \\ & \text{O} & \text{O} & \text{O} & \text{O} \\ & \text{O} & \text{O} & \text{O} & \text{O} \\ & \text{O} & \text{O} & \text{O} & \text{O} \\ & \text{O} & \text{O} & \text{O} & \text{O} \\ & \text{O} & \text{O} & \text{O} & \text{O} \\ & \text{O} \\ & \text{O} \\ & \text{O} & \text{O} \\ & \text{O}$$

RN 153685-17-7 CAPLUS

CN 3-Pyridinecarboxamide, N-[[3-[(butylamino)carbonyl]phenyl]sulfonyl]-6-(ethoxymethyl)- (9CI) (CA INDEX NAME)

RN 153685-18-8 CAPLUS

CN 3-Pyridinecarboxamide, N-[[2-chloro-5-[[[2-(4-fluorophenyl)ethyl]amino]carbonyl]phenyl]sulfonyl]-6-(hydroxymethyl)-, monoammonium salt (9CI) (CA INDEX NAME)

NH3

RN 153685-19-9 CAPLUS

CN 3-Pyridinecarboxamide, N-[[4-[2-[(cyclohexylacetyl)amino]ethyl]phenyl]sulf onyl]-6-(hydroxymethyl)-, monoammonium salt (9CI) (CA INDEX NAME)

● NH3

RN 153685-20-2 CAPLUS

CN 3-Pyridinecarboxamide, 6-(hydroxymethyl)-N-[[4-[2-[(2-methyl-1-oxopropyl)amino]ethyl]phenyl]sulfonyl]-, monoammonium salt (9CI) (CA INDEX NAME)

● инз

RN 153685-21-3 CAPLUS

CN 3-Pyridinecarboxamide, N-acetyl-6-[(acetyloxy)methyl]-N-[[4-[2-[(2-chloro-5-methoxybenzoyl)amino]ethyl]phenyl]sulfonyl]- (9CI) (CA INDEX NAME)

L10 ANSWER 41 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1994:100174 CAPLUS

DN 120:100174

Novel inhibitors of prolyl 4-hydroxylase. 5. The intriguing structure-activity relationships seen with 2,2'-bipyridine and its 5,5'-dicarboxylic acid derivatives

AU Hales, Neil J.; Beattie, John F.

CS Infect. Res. Dep., Zeneca Pharm., Macclesfield/Cheshire, SK10 4TG, UK

SO Journal of Medicinal Chemistry (1993), 36(24), 3853-8 CODEN: JMCMAR; ISSN: 0022-2623

DT Journal

LA English

AB Members of a series of 2,2'-bipyridines have been synthesized and tested as inhibitors of prolyl hydroxylase (EC 1.14.11.2). The structure-activity relationships seen with [2,2'-bipyridine]-5-carboxylic acid (I) closely resemble those of pyridine-2-carboxylic acid (II). Accordingly, [2,2'-bipyridine]-5,5'-dicarboxylic acid (III, IC50 = 0.19 μM) is the most potent inhibitor of its type yet reported. However, 2,2'-bipyridines lacking a 5-carboxylate are poor inhibitors. These contrasting structure-activity relationships are discussed in terms of net anionic charge, iron chelation, and the availability of alternative putative binding modes at a single binding site in each catalytic subunit. This series of inhibitors may provide insight for the design of drugs effective in the inhibition of excess collagen deposition.

IT 152365-37-2P 152365-39-4P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of and prolyl hydroxylase inhibition by, structure in relation to)

RN 152365-37-2 CAPLUS

CN [2,2'-Bipyridine]-5-carboxamide, N-(phenylsulfonyl)- (9CI) (CA INDEX NAME)

RN 152365-39-4 CAPLUS

CN [2,2'-Bipyridine]-5,5'-dicarboxamide, N,N'-bis(phenylsulfonyl)- (9CI) (CA INDEX NAME)

L10 ANSWER 42 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1993:671084 CAPLUS

DN 119:271084

TI 2-(Alkylamino)nicotinic acid and analogs. Potent angiotensin II antagonists

AU Winn, Martin; De, Biswanath; Zydowsky, Thomas M.; Altenbach, Robert J.; Basha, Fatima Z.; Boyd, Steven A.; Brune, Michael E.; Buckner, Steven A.; Crowell, DeAnne; et al.

CS Cardiovas. Res. Div., Abbott Lab., Abbott Park, IL, 60064, USA

SO Journal of Medicinal Chemistry (1993), 36(18), 2676-88 CODEN: JMCMAR; ISSN: 0022-2623

DT Journal

LA English

AB A series of pyridines and other six-membered ring heterocycles connected to a biphenyl-tetrazole with a -CH2-NR1-link were discovered to be potent angiotensin II antagonists. In the pyrimidine carboxylic acid series I (W = CR, X = N, Y = CH, Z = COOH), compds. with an alkyl group (R1) on the exocyclic nitrogen were much more potent than compds. with an alkyl group (R) on the heterocyclic ring. The corresponding pyridine, pyridazine, pyrazine, and 1,2,4-triazine carboxylic acids also showed potent in vitro angiotensin II antagonism. The pyridine I (W, X, Y = CH, Z = COOH, R1 = n-C3H7) demonstrated potent in vitro activity (pA2 = 10.10, rabbit aorta, and Ki = 0.61 nM, receptor binding in rat liver) as well as exceptional oral antihypertensive activity and bioavailability. Any nonacidic replacement for the carboxylic acid was detrimental for activity.

IT 151323-15-8P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation and angiotensin II antagonist activity of)

RN 151323-15-8 CAPLUS

CN 3-Pyridinecarboxamide, N-(phenylsulfonyl)-2-[propyl[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]amino]- (9CI) (CA INDEX NAME)

IT 151323-51-2P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

RN 151323-51-2 CAPLUS

CN 3-Pyridinecarboxamide, N-(phenylsulfonyl)-2-[propyl[[2'-[2-(triphenylmethyl)-2H-tetrazol-5-yl][1,1'-biphenyl]-4-yl]methyl]amino]-

(9CI) (CA INDEX NAME)

- L10 ANSWER 43 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
- AN 1993:254964 CAPLUS
- DN 118:254964
- TI Preparation of (pyridylthio- or pyridyloxy)pyrimidine or -triazine derivatives as herbicides
- IN Miyazaki, Masahiro; Matsuzawa, Masafumi; Toriyabe, Keiji; Hirata, Michiya
- PA Kumiai Chemical Industry Co., Ltd., Japan; Ihara Chemical Industry Co., Ltd.
- SO PCT Int. Appl., 77 pp. CODEN: PIXXD2
- DT Patent
- LA Japanese
- FAN CNT 2

FAN.		TENT NO.			KINI						PLICATION NO.		DATE
PI	WO				A 1		1992	1015		WO	1992-JP362		19920326
											R, IT, LU, MC,	NL.	SE
	JР	05331163	22,	J,	A2	,	1993	1214	02,	JP	1991-84556	,	19910326
	CA	2078336			AA		1992	0927		CA	1991-84556 1992-2078336		19920326
	AU	9214517			A1		1992	1102		AU	1992-14517		19920326
	AU	645193			В2		1994	0106					
	ΕP	532761			A1		1993	0324		ΕP	1992-907592		19920326
		R: AT,	BE,	CH,	DE,	DK,	, ES,	FR,	GB,	, G	R, IT, LI, LU,	MC,	NL, SE
	HU	62761			A2		1993	0628		HU	1992-3716		19920326
	HU	62761 212644			В		1996	0930					
	BR	9204796			Α		1993	0831		BR	1992-4796		19920326
		2066321									1992-16418		
	PL	171471			В1		1997	0530		PL	1992-296936		19920326
	RO	112112			B1		1997	0530		RO	1992-1473 1992-CA402		19920326
	IN	174958			Α		1995	0408		IN	1992-CA402		19920604
	IN	175877			Α		1995	1014		IN	1992-CA401 1992-105035		19920604
		1080637			Α		1994	0112		CN	1992-105035		19920622
		1080638			Α		1994 1998 1995	0112		CN	1992-105045		
		1040280			В		1998	1021					
	US	5385880			Α		1995	0131		US	1992-927281		19920917
	IN	178208 178419			A		1997				1994-CA798		
	IN	178419			A		1997			IN	1994-CA799		19940930
PRAI		1991-845											
		1992-JP3											
		1992-CA4											
00		1992-CA4		<i>c</i> 1	A1		1992	0004					
os	MAIM	RPAT 118:	∠349	04									

AB The title compds. [I; R = H, HO, alkoxy, alkoxyalkoxy, acyloxyalkoxy, (un)substituted PhCH2O, Me3SiCH2CH2O, etc.; R1, R2 = H, alkoxy, halo, (di)alkylamino, haloalkoxy, alkyl; W = O, S, NH, N(CHO), alkoxycarbonylimino; Z = CH, N; X = halo, (halo)alkyl, acylamino, (halo)cycloalkyl, alkenyloxy, alkynyloxy, (un)substituted Ph or PhCH2, etc.] are prepared Thus, sulfonylation of Me 2-hydroxy-4-phenylnicotinate with (CF3SO2)2O in CH2Cl2 at -20° to -10° followed by condensation with 4,6-dimethoxy-2-hydroxypyrimidine in the presence of K2CO3 in DMSO at 80° gave a pyrimidine derivative (II; R = OMe) which was hydrolyzed to II (R = OH). This at 100 g/10 are in paddy field soil controlled ≥90% Echinochloa crus-galli, Monochoria vaginalis, and Scirpus juncoides. A total of 173 I were prepared

IT 147078-07-7P

RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic



preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (preparation of, as herbicide)

RN 147078-07-7 CAPLUS

CN 3-Pyridinecarboxamide, 4-(3-chlorophenyl)-2-[(4,6-dimethoxy-2-pyrimidinyl)thiol-N-(methylsulfonyl)- (9CI) (CA INDEX NAME)

L10 ANSWER 44 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1993:49068 CAPLUS

DN 118:49068

TI New type antifoggants for silver halide photographic materials. II

AU Shibuya, Isao; Yonemoto, Katsumi; Kaneko, Yutaka; Hirabayashi, Shigeto; Taguchi, Yoichi; Tsuchiya, Tohru; Yasumoto, Masahiko

CS Natl. Chem. Lab. Ind., Tsukuba, Japan

SO Nippon Shashin Gakkaishi (1992), 55(4), 248-53 CODEN: NSGKAP; ISSN: 0369-5662

DT Journal

LA Japanese

AB In the study on organic functional materials, >100 compds. containing S and/or

N

atoms, such as S-(disubstituted thiocarbamoyl)-N-(substituted formyl) sulfenamides, and their related compds., S-(disubstituted thiocarbamoyl) thiooximes, and various heterocycles, were newly prepared Their antifogging activity for color photog. were examined The thiooximes as well as the sulfenamides are excellent antifoggants superior to conventional ones. Their skeletal structure which has a C=S group and its neighboring N is responsible for their antifogging activity.

IT 138906-05-5

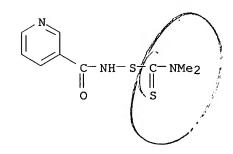
RL: USES (Uses)

(photog. antifogging characteristics of)

RN 138906-05-5 CAPLUS

CN 3-Pyridinecarboxamide, N-[[(dimethylamino)thioxomethyl]thio]- (9CI) (CA

INDEX NAME)



L10 ANSWER 45 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1992:255548 CAPLUS

DN 116:255548

TI Preparation of 1,4,2-dithiazolium salts

AU Yonemoto, Katsumi; Shibuya, Isao; Taguchi, Yoichi; Tsuchiya, Tohru; Yasumoto, Masahiko

CS Natl. Chem. Lab. Ind., Tsukuba, 305, Japan

SO Bulletin of the Chemical Society of Japan (1992), 65(3), 920-2 CODEN: BCSJA8; ISSN: 0009-2673

DT Journal

LA English

OS CASREACT 116:255548

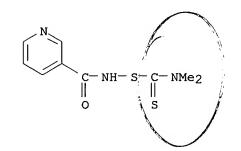
AB R2NCSSNHCOR1 I [R2N = Me2N, Et2N, (Me2CH)2N, piperidino; R1 = Me3C, Me, 2-thienyl, 3-pyridyl, Et2N, MeO] were treated with a strong acid (HBF4 or HClO4) in Ac2O to afford 1,4,2-dithiazolium salts II (X- = BF4-, ClO4-) and/or 1,2,4-trithiolanebisdialkyliminium salts III. The reactivity is markedly dependent on the nature of substituents (NR2 and R1) and the acid used. I (R2N = Me2N, Et2N, R1 = MeO) reacted successively with NaH and p-toluenesulfonyl chloride to give (R2NCS2)2NCO2Me (IV). The mechanisms for the formation of III and IV are discussed.

IT 138906-05-5

RL: RCT (Reactant); RACT (Reactant or reagent)
 (intramol. cyclocondensation of, dithiazolium and trithiolanediiminium
 salts from)

RN 138906-05-5 CAPLUS

CN 3-Pyridinecarboxamide, N-[[(dimethylamino)thioxomethyl]thio]- (9CI) (CA INDEX NAME)





L10 ANSWER 46 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1992:128199 CAPLUS

DN 116:128199

TI Preparation of thiocarbamoylsulfenamides

IN Yonemoto, Katsumi; Shibuya, Isao

PA Agency of Industrial Sciences and Technology, Japan

SO Jpn. Kokai Tokkyo Koho, 4 pp. CODEN: JKXXAF

DT Patent

LA Japanese

FAN. CNT 1

TAN. ON I								
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE				
PI JP 03236369	A2	19911022	JP 1990-32214	19900213				
JP 05052824	B4	19930806						
PRAI JP 1990-32214		19900213						

OS CASREACT 116:128199; MARPAT 116:128199

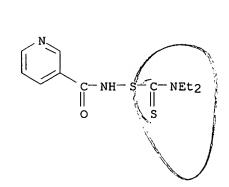
AB R2R3NC(S)SNHCOR1 (I; R1 = aryl, heterocycle, alkyl, dialkylamino, alkoxy; R2, R3 = lower alkyl; NR2R3 may form ring) are prepared by treating R1CONH2 (R1 = same as I) with NaH and iodine followed by R2R3NC(S)S-M+ (R2, R3 = same as I; M = metal). Me carbamate in THF was treated with NaH followed by iodine, Et2NC(S)S-Ag+ was added, and the mixture was stirred for 30 min to give 87% I (R1 = OMe, R2 = R3 = Et).

IT 138906-04-4P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of, by condensation of amide with dithiocarbamate)

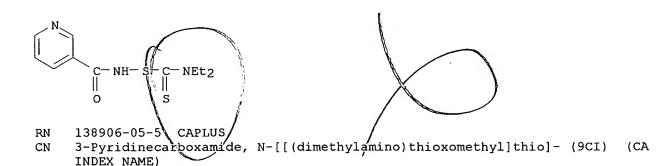
RN 138906-04-4 CAPLUS

CN 3-Pyridinecarboxamide, N-[[(diethylamino)thioxomethyl]thio]- (9CI) (CA INDEX NAME)





- L10 ANSWER 47 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
- AN 1992:83195 CAPLUS
- DN 116:83195
- TI Preparation of N-(substituted formyl)dialkylamino(thioxo)methanesulfenamid es
- AU Yonemoto, Katsumi; Shibuya, Isao; Yasumoto, Masahiko; Taguchi, Yoichi; Tsuchiya, Tohru
- CS Natl. Chem. Lab. Ind., Tsukuba, 305, Japan
- SO Bulletin of the Chemical Society of Japan (1991), 64(12), 3732-4 CODEN: BCSJA8; ISSN: 0009-2673
- DT Journal
- LA English
- OS CASREACT 116:83195
- AB Methanesulfenamides R2NCS2NHCOR1 (R2N = Et2N, Me2N, piperidino, morpholino; R1 = alkyl, dialkylamino, alkoxy, aryl, heteroaryl, H, styryl), antifoggants for silver halide photog. materials as well as potential precursors for 1,4,2-dithiazolium salts, were prepared in good yields in two one-pot procedures. Various amide-type compds. R2CONH2 were treated successively with NaH and I2 and then condensed with dialkyldithiocarbamates (Method A); or R2CONH2 were reacted with tetraalkylthiuram disulfides after treatment with NaH (Method B).
- IT 138906-04-4P 138906-05-5P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
- RN 138906-04-4 CAPLUS
- CN 3-Pyridinecarboxamide, N-[[(diethylamino)thioxomethyl]thio]- (9CI) (CA INDEX NAME)



L10 ANSWER 48 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1991:553116 CAPLUS

DN 115:153116

TI Preparation of fluoroethylsulfonamides as insecticides and acaricides.

IN Mori, Kaoru; Komata, Takeo; Tamai, Ryoichi; Murakami, Kazuko; Tada, Osamu; Koyasu, Hideo; Matsubuchi, Sadayuki; Fujisawa, Toyoichi

PA Central Glass Co., Ltd., Japan; Kumiai Chemical Industry Co., Ltd.

SO Jpn. Kokai Tokkyo Koho, 13 pp. CODEN: JKXXAF

DT Patent

LA Japanese

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI PRAI	JP 03068550 JP 1989-206276	A2	19910325 19890809	JP 1989-206276	19890809

OS MARPAT 115:153116

AB R1SO2NR2CH2CH2F [I; R1 = C1-4 alkyl, haloalkyl, thienyl, C6H4Xm; R2 = C1-4 alkyl, alkynyl, haloalkyl, cycloalkyl, OCH2Ph, SO2Ph, COR3; R3 = C1-6 alkyl, alkynyl, haloalkyl, (haloalkyl)cycloalkyl, (halo)benzyl, C1-6 alkoxy, alkenyloxy, OPh, NHPh, (halo)pyridyl, naphthyl, furyl, C6H4Yn; X = H, halo, C1-4 alkyl, haloalkyl, alkoxy, nitro, cyano; Y = X, amino; m, n = 1-2] are prepared as insecticides or acaricides. N-(2-Fluoroethyl)-3-toluenesulfonamide (preparation given) in THF was treated with NaH at room temperature for 1 h, mixed with BzCl, and stirred at room temperature overnight to

give 76.4% I (R1 = 3-MeC6H4, R2 = Bz), which was applied to cucumber at 4 ppm to control Aphis gossypii with 100% mortality.

IT 136160-60-6P 136161-38-1P 136161-39-2P

RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of, as insecticide and acaricide)

RN 136160-60-6 CAPLUS

CN 3-Pyridinecarboxamide, N-(2-fluoroethyl)-N-(phenylsulfonyl)- (9CI) (CA INDEX NAME)

RN 136161-38-1 CAPLUS

CN 3-Pyridinecarboxamide, 2-chloro-N-(2-fluoroethyl)-N-(phenylsulfonyl)-(9CI) (CA INDEX NAME)

$$\begin{array}{c|c}
 & C1 & O \\
 & O & S-Ph \\
 & C-N-CH_2-CH_2F \\
 & O & O
\end{array}$$

RN 136161-39-2 CAPLUS
CN 3-Pyridinecarboxamide, 6-chloro-N-(2-fluoroethyl)-N-(phenylsulfonyl)(9CI) (CA INDEX NAME)

$$\begin{array}{c|c}
\text{Cl} & \text{N} & \text{O} \\
\text{O} & \text{S-Ph} \\
\text{C-N-CH}_2\text{-CH}_2\text{F} \\
\text{O}
\end{array}$$

L10 ANSWER 49 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1991:192389 CAPLUS

DN 114:192389

TI Improved delivery through biological membranes. 46. Synthesis, characterization and in vitro evaluation of various sulfonamide chemical delivery systems

AU Brewster, Marcus E.; Deyrup, Margaret; Seyda, Kazimierz; Bodor, Nicholas

CS Coll. Pharm., Univ. Florida, Gainesville, FL, 32610, USA

SO International Journal of Pharmaceutics (1991), 68(1-3), 215-29 CODEN: IJPHDE; ISSN: 0378-5173

DT Journal

LA English

Dihydropyridine .dblarw. pyridinium salt type chemical delivery systems were prepared for several sulfonamides found useful in the treatment of cerebral toxoplasmosis. Sulfadiazine, sulfamethoxazole, sulfamerazine, and sulfamethazine were considered and both aniline (N4) and sulfamide (N1) derivatization were performed. The sulfamethoxazole derivative in which a reduced nicotinamide moiety was attached at the N1 site provided a compound which rapidly oxidized in various matrixes and was highly lipophilic. In addition, studies in rat brain homogenates illustrated appropriate conversion of the chemical delivery system with ultimate release of the active sulfa drug.

IT 133411-94-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and quaternization of)

RN 133411-94-6 CAPLUS

CN 3-Pyridinecarboxamide, N-[(4-aminophenyl)sulfonyl]-N-(5-methyl-3-isoxazolyl)- (9CI) (CA INDEX NAME)

IT 133411-95-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reduction of)

RN 133411-95-7 CAPLUS

CN Pyridinium, 3-[[[(4-aminophenyl)sulfonyl](5-methyl-3-isoxazolyl)amino]carbonyl]-1-methyl-, iodide (9CI) (CA INDEX NAME)

• I-

L10 ANSWER 50 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1990:178928 CAPLUS

DN 112:178928

TI Synthesis of some pyrido[2,3-c][1,2,6]triazonine derivatives

AU Soloducho, Jadwiga

CS Inst. Org. Phys. Chem., Tech. Univ. Wroclaw, Wroclaw, PL-50-370, Pol.

SO Journal fuer Praktische Chemie (Leipzig) (1989), 331(3), 503-6 CODEN: JPCEAO; ISSN: 0021-8383

DT Journal

LA English

OS CASREACT 112:178928

Treating nicotinic acid derivative I (R = tosyl) with K, followed by treatment of the product with Br(CH2)3Br gave 81% pyridotriazonine II (R1= R3 = tosyl, R2 = H) (III). Hydrolysis of III with 48% H2SO4 gave II (R1-R3 = H) (IV). Mannich reaction of IV with formaldehyde and morpholine or piperidine gave II (R1 = R2 = H, R3 = CH2R4; R4 = morpholino, piperidino). Alkylation of IV with ClCH2CH2NEt2 gave II (R1 = R3 = H, R2 = CH2CH2NEt2).

IT 109274-64-8

RL: RCT (Reactant); RACT (Reactant or reagent) (sequential metalation and cyclocondensation reaction with dibromopropane, pyridotriazonine derivative from)

RN 109274-64-8 CAPLUS

CN Benzenesulfonic acid, 4-methyl-, 2-[3-[[[(4-methylphenyl)sulfonyl]amino]carbonyl]-2-pyridinyl]hydrazide (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} R - C - NH - S \\ \parallel & \parallel \\ O & O \end{array}$$

L10 ANSWER 51 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1988:131590 CAPLUS

DN 108:131590

TI Preparation of (phenylsulfonyl)nicotinamide derivatives as agricultural fungicides

IN Yoshida, Hiroshi; Koike, Kengo; Konishi, Kenji; Shimano, Shizuo; Nakagawa, Taizo

PA Nippon Kayaku Co., Ltd., Japan

SO Jpn. Kokai Tokkyo Koho, 6 pp. CODEN: JKXXAF

DT Patent

LA Japanese

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
ΡI	JP 62181261	A2	19870808	JP 1986-22999	19860206
PRAT	JP 1986-22999		19860206		

AB The title compds. (I; X = H, halo, MeS; Y = H, halo, Me, MeO, CF3, MeS; n = 1-3), useful as agricultural fungicides, were prepared A mixture of 4-MeC6H4SO2NH2 and 2-chloronicotinoyl chloride in pyridine was stirred for 2 h at room temperature to give 48.4% I (X = 2-Cl, Yn = 4-Me). At 200 ppm, I

(X = H, Yn = 4-Me) provided 72% protection to rice plants against Pyricularia oryzae. A formulation containing 2 parts I (X = H, Yn = 2-Me) and 98 parts clay was prepared

IT 113513-61-4P 113513-62-5P 113513-63-6P 113513-64-7P 113513-65-8P 113513-66-9P

113513-67-0P 113513-68-1P 113513-69-2P

113513-70-5P 113513-71-6P 113513-72-7P

113513-73-8P 113513-74-9P 113513-75-0P

113513-76-1P 113513-77-2P 113513-78-3P

113513-79-4P 113513-80-7P 113513-81-8P

113513-82-9P 113513-83-0P

RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of, as agricultural fungicide)

RN 113513-61-4 CAPLUS

CN 3-Pyridinecarboxamide, N-[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)

RN 113513-62-5 CAPLUS

CN 3-Pyridinecarboxamide, N-[(2-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)

RN 113513-63-6 CAPLUS

CN 3-Pyridinecarboxamide, 2-chloro-N-[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)

RN 113513-64-7 CAPLUS

CN 3-Pyridinecarboxamide, 2-chloro-N-[(2-chlorophenyl)sulfonyl]- (9CI) (CA INDEX NAME)

RN 113513-65-8 CAPLUS

CN 3-Pyridinecarboxamide, 2-chloro-N-[(2-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)

RN 113513-66-9 CAPLUS

CN 3-Pyridinecarboxamide, 2-chloro-N-[(2-fluorophenyl)sulfonyl]- (9CI) (CA INDEX NAME)

RN 113513-67-0 CAPLUS

CN 3-Pyridinecarboxamide, 2-chloro-N-(phenylsulfonyl)- (9CI) (CA INDEX NAME)

RN 113513-68-1 CAPLUS

CN 3-Pyridinecarboxamide, 2-chloro-N-[(4-fluorophenyl)sulfonyl]- (9CI) (CA INDEX NAME)

RN 113513-69-2 CAPLUS

CN 3-Pyridinecarboxamide, 6-chloro-N-[(2,4,5-trichlorophenyl)sulfonyl]- (9CI) (CA INDEX NAME)

RN 113513-70-5 CAPLUS

CN 3-Pyridinecarboxamide, 6-chloro-N-[(4-methoxyphenyl)sulfonyl]- (9CI) (CA INDEX NAME)

RN 113513-71-6 CAPLUS

CN 3-Pyridinecarboxamide, 4-chloro-N-[(4-fluorophenyl)sulfonyl]- (9CI) (CA INDEX NAME)

RN 113513-72-7 CAPLUS

CN 3-Pyridinecarboxamide, N-(phenylsulfonyl)- (9CI) (CA INDEX NAME)

RN 113513-73-8 CAPLUS

CN 3-Pyridinecarboxamide, N-[(4-methylphenyl)sulfonyl]-2-(methylthio)- (9CI) (CA INDEX NAME)

RN 113513-74-9 CAPLUS

CN 3-Pyridinecarboxamide, 5-bromo-N-[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)

RN 113513-75-0 CAPLUS

CN 3-Pyridinecarboxamide, N-[(4-chloro-2-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)

RN 113513-76-1 CAPLUS

CN 3-Pyridinecarboxamide, N-[(4-chlorophenyl)sulfonyl]- (9CI) (CA INDEX NAME)

RN 113513-77-2 CAPLUS

CN 3-Pyridinecarboxamide, 5-bromo-N-[[3-(trifluoromethyl)phenyl]sulfonyl]- (9CI) (CA INDEX NAME)

RN 113513-78-3 CAPLUS

CN 3-Pyridinecarboxamide, N-[[4-chloro-2-(trifluoromethyl)phenyl]sulfonyl]-2-(methylthio)- (9CI) (CA INDEX NAME)

RN 113513-79-4 CAPLUS

CN 3-Pyridinecarboxamide, 2-(methylthio)-N-[[4-(methylthio)phenyl]sulfonyl]-(9CI) (CA INDEX NAME)

RN 113513-80-7 CAPLUS

CN 3-Pyridinecarboxamide, 2-(methylthio)-N-[[3-(trifluoromethyl)phenyl]sulfon yl]- (9CI) (CA INDEX NAME)

RN 113513-81-8 CAPLUS

CN 3-Pyridinecarboxamide, N-[[4-(methylthio)phenyl]sulfonyl]- (9CI) (CA INDEX NAME)

RN 113513-82-9 CAPLUS

CN 3-Pyridinecarboxamide, N-[[4-chloro-2-(trifluoromethyl)phenyl]sulfonyl]- (9CI) (CA INDEX NAME)

RN 113513-83-0 CAPLUS
CN 3-Pyridinecarboxamide, 6-chloro-N-[(4-fluorophenyl)sulfonyl]- (9CI) (CA INDEX NAME)

L10 ANSWER 52 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1987:459010 CAPLUS

DN 107:59010

TI Synthesis of some pyrido[3,2-g][1,2,5]triazocine derivatives

AU Soloducho, Jadwiga

CS Dep. Technol. Drugs, Sch. Med., Wroclaw, 50140, Pol.

SO Polish Journal of Chemistry (1986), 59(10-12), 1115-20 CODEN: PJCHDQ; ISSN: 0137-5083

DT Journal

LA English

OS CASREACT 107:59010

AB The title compds. I (R = H, morpholinomethyl, piperidinomethyl; R1 = H, Et2NCH2CH2, 2-hydroxy-3-morpholinopropyl) were prepared starting from 2-chloronicotinamide.

IT 109274-64-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and cyclocondensation of, with dibromomethane)

RN 109274-64-8 CAPLUS

CN Benzenesulfonic acid, 4-methyl-, 2-[3-[[[(4-methylphenyl)sulfonyl]amino]carbonyl]-2-pyridinyl]hydrazide (9CI) (CA INDEX NAME)

IT 109274-70-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reaction of, with dibromoethane)

RN 109274-70-6 CAPLUS

CN Benzenesulfonic acid, 4-methyl-, 2-[3-[[[(4-methylphenyl)sulfonyl]amino]carbonyl]-2-pyridinyl]hydrazide, monopotassium salt (9CI) (CA INDEX NAME)

● K

L10 ANSWER 53 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1983:198028 CAPLUS

DN 98:198028

TI Pyridine derivatives inducing tillering and agricultural compositions containing them

IN Stacey, Gilbert Joseph; Hawkins, Alan Francis; Pearson, David Philip John; Sunley, Raymond Leo

PA Imperial Chemical Industries PLC, UK

SO Eur. Pat. Appl., 40 pp. CODEN: EPXXDW

DT Patent

LA English

FAN.CNT 1

FAIV.	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 67511	A2	19821222	EP 1982-302208	19820429
	EP 67511	A3	19830406		
	R: AT, BE, CH,	DE, FR	, GB, IT, LI	, LU, NL, SE	
	GB 2099421	Α	19821208	GB 1982-12420	19820419
	AU 8283671	A1	19821125	AU 1982-83671	19820513
	US 4473395	Α	19840925	US 1982-379047	19820517
	ES 512295	A1	19830201	ES 1982-512295	19820518
	BR 8202876	Α	19830426	BR 1982-2876	19820518
	JP 57197267	A2	19821203	JP 1982-83339	19820519
PRAI	GB 1981-15251	Α	19810519		
	GB 1981-15252	Α	19810519		
	GB 1981-24941	Α	19810814		
	GB 1982-12420	Α	19820419		
	EP 1982-302208	Α	19820429		
os	CASREACT 98:198028;	MARPAT	98:198028		

AB Phenylpyridine I [R = Ph, substituted Ph; Rl = cyano, carboxy, alkoxycarbonyl, alkylthiocarbonyl, carbamoyl; R2 = H, halogen, (un)substituted alkyl, OH, NH2, Ph, alkoxycarbonyl; n = 0, 1] were prepared Thus 4-ClC6H4CH2CO2H was treated with POCl3-DMF to give Me2NCH:C(CHO)C6H4Cl-4, which was cyclized with H2NCMe:CHCO2Et to form I (R = C6H4Cl-4; R1 = CO2Et; R2 = Me, n = 0)(II). II gave 132% of control barley tillering at 3 kg/ha.

IT 85582-91-8P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation and tillering-inducing activity of)

RN 85582-91-8 CAPLUS

CN 3-Pyridinecarboxamide, 5-(4-chlorophenyl)-2-methyl-N-(methylsulfonyl)-(9CI) (CA INDEX NAME)

No Wielity

L10 ANSWER 54 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1981:550092 CAPLUS

DN 95:150092

- TI Participation of electrophilic organic compounds of sulfur(II) in catalytic conversions. III. Certain features of the synthesis and chemical behavior of N-acyl derivatives of 2-nitrobenzenesulfenic acid amide
- AU Parfenov, E. A.; Fomin, V. A.; Maksimova, A. A.
- CS Vses. Nauchno-Issled. Vitam. Inst., Moscow, USSR
- SO Zhurnal Obshchei Khimii (1981), 51(5), 1137-44 CODEN: ZOKHA4; ISSN: 0044-460X

DT Journal

LA Russian

AB Reaction of 2-O2NC6H4SCl (I) with H2NCHO in the presence of Et3N and DMF gave 2-O2NC6H4SNHCHO (II), (2-O2NC6H4S)2NCHO and (2-O2NC6H4S)2 (III). I and excess H2NCHO gave II, III and (2-O2NC6H4S)2NH. Similar results were obtained with nicotinamide. Activation of the S-N bond under conditions of basic catalysis was a necessary but insufficient condition for the substitution of a sulfenic acid residue in a sulfenated amine by an acyl group from S-esters of thiocarboxylic acids. The probability of substitution increased with increasing basicity of the sulfenated amine.

TT 79352-15-1P 79352-16-2P
RI: SPN (Synthetic preparation):

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

RN 79352-15-1 CAPLUS

CN 3-Pyridinecarboxamide, N-[(2-nitrophenyl)thio]- (9CI) (CA INDEX NAME)

RN 79352-16-2 CAPLUS

CN 3-Pyridinecarboxamide, N,N-bis[(2-nitrophenyl)thio]- (9CI) (CA INDEX NAME)

L10 ANSWER 55 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1976:523526 CAPLUS

DN 85:123526

TI Reaction of norsulfazole and sulfadimezine with aromatic carboxylic acids

AU Kalashnikov, V. P.; Turkevich, N. M.

CS L'vov. Med. Inst., Lvov, USSR

SO Farmatsiya (Moscow, Russian Federation) (1976), 25(4), 38-41 CODEN: FRMTAL; ISSN: 0367-3014

DT Journal

LA Russian

AB Reaction of norsulfazole (I) with o-HOC6H4CO2H gave 60% p-(o-HOC6H4CO)2NC6H4SO2NRCOC6H4OH-o (R=2-thiazolyl); similar results were obtained by reaction of I with nicotinic acid. Reaction of I with o-AcOC6H4CO2H gave 70% p-H2NC6H4SO2NRCOC6H4OAc-o. Treatment of sulfadimesine with o-R1OC6H4CO2H (R1=Ac,H) gave p-H2NC6H4SO2NR2COC6H4OR1-o (R2=4,6-dimethyl-2-pyrimidenyl) in 61 and 65% yield, resp.

IT 60671-86-5P

RN 60671-86-5 CAPLUS

CN 3-Pyridinecarboxamide, N-[[4-[bis(3-pyridinylcarbonyl)amino]phenyl]sulfony 1]-N-2-thiazolyl- (9CI) (CA INDEX NAME)

L10 ANSWER 56 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1975:458608 CAPLUS

DN 83:58608

TI Synthesis and pharmacological properties of some N-acylsulfonamides

AU Delarge, J.; Lapiere, C. L.

CS Inst. Pharm., Univ. Liege, Liege, Belg.

SO Annales Pharmaceutiques Francaises (1974), 32(12), 657-67 CODEN: APFRAD; ISSN: 0003-4509

DT Journal

LA French

OS CASREACT 83:58608

AB Pyridinesulfonamides I (R = 3-CF3C6H4, 2-CF3C6H4, 3-ClC6H4, 4-ClC6H4, 2,3-Me(Cl)C4H3, 3-O2NC6H4, 4-O2NC6H4, 2,3-Cl2C6H3, 2,4-Cl2C6H3, 2,5-Cl2C6H3, 2,6-Cl2C6H3, 3,4-Cl2C6H3, 3,5-Cl2C6H3; R1 = H, CHO, Ac, COEt, COPr, Bz, nicotinoyl, 2-thenoyl) (39 compds.) were prepared by aminating chloropyridinesulfonamides or anilinopyridinesulfonic acids, or acylating anilinopyridinesulfonamides. II (R2 = H, Me, Et, Ph) (10 compds.) were obtained as by products. Some I and II showed diuretic activity comparable that of furosemide and antiinflammatory activity comparable to that of common antiinflammatory agents.

IT 56175-89-4P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation and antiinflammatory and diuretic activity of)

RN 56175-89-4 CAPLUS

CN 3-Pyridinecarboxamide, N-[[4-[[3-(trifluoromethyl)phenyl]amino]-3-pyridinyl]sulfonyl]- (9CI) (CA INDEX NAME)

- L10 ANSWER 57 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
- AN 1974:3511 CAPLUS
- DN 80:3511
- TI Derivatives of penam-3-carboxylic acids and cephem-4-carboxylic acids
- IN Fechtig, Bruno; Kocsis, Karoly; Bickel, Hans
- PA Ciba-Geigy A.-G.
- SO Ger. Offen., 78 pp.
- CODEN: GWXXBX
- DT Patent
- LA German
- FAN. CNT 1

FAN.	CNT I				
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
ΡI	DE 2312330	A1	19731004	DE 1973-2312330	19730313
	СН 560705	A	19750415	CH 1972-4251	19720322
	ZA 7301905	Α	19731219	ZA 1973-1905	19730319
	DD 105617	С	19740512	DD 1973-169591	19730320
	AU 7353499	A1	19740926	AU 1973-53499	19730320
	ES 412838	A1	19760516	ES 1973-412838	19730320
	CA 1049501	A1	19790227	CA 1973-166491	19730320
	BE 797084	A1	19730921	BE 1973-129044	19730321
	FR 2181839	A1	19731207	FR 1973-10084	19730321
	AT 7302519	Α	19750115	AT 1973-2519	19730321
	AT 325765	В	19751110		
	AT 7408632	Α	19750315	AT 1974-8632	19730321
	ни 169031	P	19760928	HU 1973-CI1355	19730321
	US 3996208	Α	19761207	US 1973-344020	19730321
	NL 7304036	Α	19730925	NL 1973-4036	19730322
	JP 49005988	A2	19740119	JP 1973-34000	19730322
	GB 1423386	Α	19760204	GB 1973-13848	19730322
	SE 7602730	Α	19760227	SE 1976-2730	19760227
PRAI	CH 1972-4251	Α	19720322		
	CH 1972-12919	Α	19720901		
	CH 1972-18530	Α	19721220		

- AB The N-sulfamylampicillins I (R = alkyl, aryl, substituted amino, N-heterocyclic) (48 compds.) were prepared by treating a trimethylsilylated ampicillin with RCONHSO2Cl. The RCONHSO2Cl were obtained by treating RCO2H with ClSO2NCO. Some related cephalosporins (3 compds.) were similarly prepared Thus, nicotinoylsulfamyl chloride, prepared by treating nicotinic acid with ClSO2NCO, was treated with trimethylsilyl N-trimethylsilyl-6-D- α -phenylglycylaminopenicillanate to give I (R = 3-pyridyl).
- IT 50881-21-5P 50881-59-9P
 - RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 - (preparation and reaction of, with ampicillin derivative)
- RN 50881-21-5 CAPLUS
- CN Sulfamoyl chloride, [(1,6-dihydro-6-oxo-3-pyridinyl)carbonyl]- (9CI) (CA INDEX NAME)

RN 50881-59-9 CAPLUS

CN Sulfamoyl chloride, [(2-chloro-3-pyridinyl)carbonyl]- (9CI) (CA INDEX NAME)

IT. 50881-62-4P 50882-05-8P 51032-26-9P

51032-28-1P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)

RN 50881-62-4 CAPLUS

CN 4-Thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid, 6-[[[[[(1,6-dihydro-6-oxo-3-pyridinyl)carbonyl]amino]sulfonyl]amino]phenylacetyl]amino]-3,3-dimethyl-7-oxo-, [2S-[2α ,5 α ,6 β (S*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 50882-05-8 CAPLUS

CN 4-Thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid, 6-[[[[[(2-chloro-3-pyridinyl)carbonyl]amino]sulfonyl]amino]phenylacetyl]amino]-3,3-dimethyl-7-oxo-, [2S-[2α , 5α , 6β (S*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 51032-26-9 CAPLUS

CN 4-Thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid, 3,3-dimethyl-7-oxo-6-[phenyl[[(3-pyridinylcarbonyl)amino]sulfonyl]amino]acetyl]amino]-, [2S-[2α , 5α , 6β (S*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 51032-28-1 CAPLUS

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
3-[(acetyloxy)methyl]-8-oxo-7-[[phenyl[[[(3-pyridinylcarbonyl)amino]sulfon yl]amino]acetyl]amino]-, [6R-[6 α ,7 β (R*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L10 ANSWER 58 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1973:58095 CAPLUS

DN 78:58095

TI N-Aroylsulfonamides

IN Moore, George G. I.; Conway, Alvin C.

PA Minnesota Mining and Manufacturing Co.

SO U.S., 4 pp. CODEN: USXXAM

DT Patent

LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
					-
PI	US 3705185	Α	19721205	US 1969-816038	19690414
PRAI	US 1969-816038	Α	19690414		

AB Twenty-three trifluoromethanesulfonamides most of them of structure I (R = F, Cl, H; R1 = NO2, CF3, halo, H; R2 = NO2, Cl, F, CN, H) or their salts, useful anticonvulsants, were prepared by treating F3CSO2NH2 and Na2CO3 (or Et3N) in Me2CO with the appropriate aroyl halide.

IT 39063-09-7P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

RN 39063-09-7 CAPLUS

CN 3-Pyridinecarboxamide, N-[(trifluoromethyl)sulfonyl]-, sodium salt (9CI) (CA INDEX NAME)

Na

L10 ANSWER 59 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

1971:405734 CAPLUS AN

75:5734 DN

ΤI Quaternary 3-pyridinium-2-quinolones

Bell, Stanley C. IN

PA American Home Products Corp.

so U.S., 4 pp. CODEN: USXXAM

Patent DT

English LΑ

FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
				
PI US 3574216	Α	19710406	US 1968-721095	19680412
PRAT US 1968-721095	Α	19680412		

Title compds., with depressant activity, were prepared Thus, 4'-chloro-2'-(2-chloro-5-sulfamoylbenzoyl)-2-iodoacetanilide,

N-(p-tolylsulfonyl)nicotinamide and Me2CO is refluxed for 24 hr and cooled to give I.

32532-10-8P 32532-12-0P IT

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)

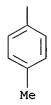
RN

32532-10-8 CAPLUS
Pyridinium, 1-[[[4-chloro-2-(2-chloro-5-sulfamoylbenzoyl)phenyl]carbamoyl] CN methyl]-3-[1-hydroxy-N-(p-tolylsulfonyl)formimidoyl]-, hydroxide, inner salt (8CI) (CA INDEX NAME)

PAGE 1-A

$$\begin{array}{c|c}
 & O \\
 & H_2N-S=0 \\
 & O \\
 & C_1 \\$$

PAGE 2-A



RN 32532-12-0 CAPLUS

CN Pyridinium, 1-[6-chloro-4-(2-chloro-5-sulfamoylphenyl)-1,2-dihydro-2-oxo-3-quinolyl]-3-[1-hydroxy-N-(p-tolylsulfonyl)formimidoyl]-, hydroxide, inner salt (8CI) (CA INDEX NAME)

L10 ANSWER 60 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1971:3525 CAPLUS

74:3525 DN

Central nervous system depressant, 1-substituted-3-[1-hydroxy-N-TI (arylsulfonyl) formimidoyl] pyridines and derivatives

IN Bell, Stanley Charles

AM HOME PA

U.S., 3 pp. SO CODEN: USXXAM

DTPatent

English LΑ

FAN CNT 1

2121	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 3534049	A	19701013	US 1968-721067	19680412

PRAI US 1968-721067 Α 19680412 The title compds. (I, R = m-AcOC6H4COCH2) (II) and (I, R = lower alkyl) (III) and the 1,2,5,6-tetrahydropyridinium (IV) and piperidinium (V) analogs of III, together with the inner salts and anion salts of I are prepared from N-(p-tolylsulfonyl)nicotinamide (VI). Thus, VI, and MeI was refluxed 18 hr in Me2CO and cooled to give III (R = Me, X = I), which was suspended in H2O and neutralized with Na2CO3 to give the inner salt of III (R = Me) (VII). VII was stirred 1 hr with aqueous NaBH4, and the mixture adjusted to pH 6 to give IV (R = Me), which was hydrogenated in H2O over 10% Pd/C to yield V (R = Me). VI and m-(BrCH2CO)C6H4OAc refluxed 2 hr in Me2CO gave II (X = Br). The compds. together with the inner salts and anion salts have central nervous system depressant and bronchodilator

activities. IT 29956-19-2P 29956-20-5P 29956-23-8P RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

RN

29956-19-2 CAPLUS
Pyridinium, 3-[1-hydroxy-N-(p-tolylsulfonyl)formimidoyl]-1-methyl-, CN hydroxide, inner salt (8CI) (CA INDEX NAME)

$$\begin{array}{c|c} Me & Me \\ \hline \\ N & N \\ \hline \\ N & N \\ \end{array}$$

RN 29956-20-5 CAPLUS

Pyridinium, 1-methyl-3-[(p-tolylsulfonyl)carbamoyl]-, iodide (8CI) (CA CN INDEX NAME)

RN

29956-23-8 CAPLUS
Pyridinium, 1-(m-hydroxyphenacyl)-3-[1-hydroxy-N-(p-tolylsulfonyl)formimidoyl]-, bromide, 1-acetate (ester) (8CI) (CA INDEX CNNAME)

PAGE 1-A

PAGE 2-A

● Br-

L10 ANSWER 61 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1963:485182 CAPLUS

DN 59:85182

OREF 59:15829d-e

TI Metabolic modifications induced by diuretic treatment and urinary elimination of some vitamins of the B complex

AU Angarano, D.; Marano, R.; Salvia, F. De

CS Univ. Bari, Italy

SO Acta Vitaminologica (1963), 17(2), 49-53 CODEN: ACVIA9; ISSN: 0001-7248

DT Journal

LA Italian

AB Not only the desired effect of diuresis was obtained in 20 patients when using thiazide compds., but also elimination of vitamins B1 and B2 and nicotinic acid in the urine of these subjects. Urine values were determined photometrically and ranged from 400 to 900 γ vitamin B1 eliminated in 24 hrs., 400 to 1120 γ vitamin B2 in 24 hrs., and 6.0 to 10 mg. of nicotinic acid in 24 hrs.

RN 856302-24-4 CAPLUS

CN 2H-1,2,4-Benzothiadiazine-7-sulfonamide, 6-chloro-, 1,1-dioxide, nicotinic acid (7CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & &$$

L10 ANSWER 62 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

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AN
     1958:55905 CAPLUS
DN
     52:55905
OREF 52:10078b-i,10079a-c
     N-Oxides and related compounds. VII. Peracid oxidation of some conjugated
     pyridines
ΑU
     Katritzky, A. R.; Monro, A. M.
     Oxford Univ., UK
CS
     Journal of the Chemical Society (1958) 150-3
SO
     CODEN: JCSOA9; ISSN: 0368-1769
DT
     Journal
     Unavailable
LA
     cf. C.A. 52, 4633d. \beta-3- and \beta-4-Pyridylacrylic acids and their
AB
     ethyl esters and amides, 2- and 4-styrylpyridines and pyridine-2-aldoxime
     and its semicarbazone gave 1-oxides with AcO2H. Pyridine (0.01 mole),
     1.47 ml. 30% aqueous H2O2, and 6 ml. AcOH was heated 18 hrs. at 70^{\circ},
     volatile matter removed at 100°/15 mm., the residue either crystallized
     directly, or if semisolid treated in 15 ml. hot CHCl3 with 0.8~\mathrm{g}. K2CO3
     and recovered from the CHCl3 by evaporation The following 1-oxides were
     prepared: \beta-4-pyridylacrylic, prisms, m. 237-40° (AmOH) (decomposition), hemiacetate, plates, m. 237-40° (AcOH) (decomposition);
     β-4-pyridylacrylamide, prisms, m. 246° (MeOH or H2O)
     (decomposition); Et \beta-4-pyridylacrylate, prisms, m. 145°
     (C6H6-petr. ether), which with 2N aqueous NaOH during 12 hrs. at 100°
     followed by AcOH gave the corresponding acid, m. 238-40°
     (decomposition), and with aqueous methanolic NH3 in 5 days at 0^{\circ} gave the
     amide, m. 245° (decomposition); \beta-3-pyridylacrylic acid, prisms m. 273-4° (AcOH) (decomposition); \beta-3-pyridylacrylamide, needles, m.
     235° (EtOH-H2O) (decomposition); Et \beta-3-pyridylacrylate, prisms, m.
     99-101° (AcOEt), also prepared by esterification of the corresponding
     acid with EtOH-H2SO4, converted (as in the 4-series) into the acid, m.
     274-5° (decomposition), and the amide, m. 235° (decomposition).
     Oxidation gave the oxide of the 2-isomer as prisms, m. 162° (C6H6),
     and the 4-isomer gave an oxide, prisms, m. 169° (MeCOEt). BzH
     (10.6 g.), 10.9 g. 2-picoline 1-oxide, and 50 ml. 5% KOMe in MeOH was
     refluxed 3 hrs., after 12 hrs. more, excess CO2 was passed in, the whole
     filtered and steam distilled yielding 22% 2-styrylpyridine 1-oxide, m.
     160°. 4-Picoline 1-oxide similarly gave 11% 4-styrylpyridine
     1-oxide, m. 167-9°. Refluxing 20.4 g. Et 3-pyridylacetate 8 hrs.
     with 11 g. KOH in 11 ml. H2O and 28 ml. EtOH followed by addition of 14.6 ml.
     aqueous 12N HCl, filtration, evaporation, and extraction of the residue with
MeOH gave
     75% 3-pyridylacetic acid, m. 141-3°; 1-oxide, prisms, m.
     142-4° (AcOEt-EtOH) (decomposition). The acid (1.27 g.), 1.5 ml. BzH,
     0.2 ml. piperidine, and 10 ml. pyridine heated 2 days at 115° and
     poured into H2O gave 40% \beta-phenyl-\alpha-3-pyridylacrylic acid,
     needles, m. 234-5° (EtOH) (decomposition). Aqueous 10% NaOH (0.5 ml.) was
     added slowly at 0° to 1.07 g. pyridine-2-aldehyde and 1.17 g.
     PhCH2CN in 2.0 ml. EtOH; after 18 hrs. 74% \alpha-phenyl-\beta-2-
     pyridylacrylonitrile was collected as prisms, m. 63-6° (EtOH).
     O-Benzoyl (pyridine-2-aldehyde cyanohydrin), prepared as the oxime benzoate
     below, formed prisms, m. 102° (EtOH). Pyridoin, needles, m.
     156°, separated later from the aqueous mother liquors. Aqueous NaCN (0.94 g.
     in 2 ml.) was added slowly at -10° to 3.14 g. quinoline-2-aldehyde
     in 10 ml. aqueous 2N HCl and the precipitated solid recrystd. (C6H6 and AcOEt)
to
     give 62% 1-cyano-1,2-di(2-quinoly1)-ethane-1,2-diol, brown plates, m.
     133° (decomposition). v Oxidation gave the aldoxime oxide, needles, m.
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222° (EtOH) (decomposition); semicarbazone oxide, insol. in CHCl3, needles, m. 233° (AcOH-AcOEt) (decomposition). Both compds. with 2,4-dinitrophenylhydrazine in alc. HCl gave the corresponding 2,4-dinitrophenylhydrazone 1-oxide, needles, m. 285-90° (AcOH) (decomposition). Extraction of crude pyridine-2-aldehyde cis-semicarbazone 1-oxide

with CHCl3 gave (from the CHCl3) 3% cis-semicarbazone, prisms, m. 158° (EtOH). On treatment with alc. HCl and 2,4dinitrophenylhydrazine, both the cis- and normal semicarbazones gave the 2,4-dinitrophenylhydrazone, m. 226-8°. BzCl (0.32 ml.) was added slowly to 0.31 g. pyridine-2-aldoxime in 1 ml. pyridine at 0°, the mixture kept 18 hrs., and H2O added yielding 80% O-benzoyl(pyridine-2aldoxime), prisms, m. 85-90° (EtOH). Treatment with AcO2H gave BzOH and pyridoin, m. 152°. 4-Acetylpyridine gave the azine, plates, m. 125.5-7° (petr. ether), and when heated 1 min. with 2 parts hydrazine hydrate yielded the hydrazone, plates, m. 121-2° (C6H6). Oxidation of 2-, 3-, and 4-(N'-benzenesulfonylhydrazinocarbonyl)p yridine gave the 4-substituted pyridine 1-oxide, needles, m. 238-9° (H2O) (decomposition), the 3-analog, needles, m. 222-4° (H2O or EtOH) (decomposition), and the 2-analog, needles, m. 209-12° (AcOH) (decomposition). Et isonicotinate (5.5 g.) was refluxed 4 hrs. with 12 ml. PhCH2NH2 and excess amine removed at 100°/14 mm. yielding 71% N-benzylisonicotinamide, needles, m. 90-2° (AcOEt-petr. ether); the methotoluene-p-sulfonate formed plates, m. 194.5-6.5° (EtOH). N-2-(3-Indoyl)ethylisonicotinamide, m. 165.5-67°, was similarly prepared by heating the amine and ester for 10 hrs. at 140° and separating from EtOH-C6H6; methotoluene-p-sulfonate, plates, m. 174-5.5° (AcOEt-EtOH). Oxidation gave pure β -4-pyridylpropionamide 1-oxide, rods, m. 227° (EtOH), and N-benzylisonicotinamide 1-oxide, prisms, m. 184° (EtOH).

IT 856639-21-9, Hydrazine, 1-nicotinoyl-1-(phenylsulfonyl)(preparation of)

RN 856639-21-9 CAPLUS

CN Hydrazine, 1-nicotinoyl-1-(phenylsulfonyl)- (6CI) (CA INDEX NAME)

L10 ANSWER 63 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1954:11402 CAPLUS

DN 48:11402

OREF 48:2118g-h

TI Penicillin salt of N, N-diethyl (thionicotinamide)

IN Rhodehamel, Harley W., Jr.

PA Eli Lilly & Co.

DT Patent

LA Unavailable

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
рT	115 2634266		19530407	US 1952-271440	19520213

AB N,N-diethyl(thionicotinamide) (I) or its salts is combined with penicillin or its salts to yield a compound of therapeutic value. I.HCl (0.3 g.) in 10 ml. H2O is added to the K salt of penicillin G (II) in 1.8 ml. H2O, and the mixture cooled and stirred occasionally to precipitate the slightly

soluble I salt

of II which is separated and dried in vacuo.

RN 882741-24-4 CAPLUS

CN INDEX NAME NOT YET ASSIGNED

CM 1

CRN 882741-23-3 CMF C10 H14 N2 O S2

CM 2

CRN 881025-87-2 CMF C16 H18 N2 O4 S

Relative stereochemistry.

L10 ANSWER 64 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1954:11401 CAPLUS

DN 48:11401 OREF 48:2118e-g

TI Antihistamine-penicillin salts

IN Short, Wallace F.; Brodrick, Charles I.; Donaldson, Margaret L.

PA Boots Pure Drug Co., Ltd.

DT Patent

LA Unavailable

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
					-
DT	CB 683400		10521126	CB 1050-3171	19500207

PI GB 683409 19521126 GB 1950-3171 19500207
AB Salts of penicillin-G (I) and basic antihistamines (II) (prepared from the

salts of penicillin-G (I) and basic antinistamines (II) (prepared from the salts of I and II by metathesis in H2O or from the free I and II by direct combination in Et2O or CHCl3) are useful where the effects of both are desired. Oily suspensions of such salts administered parenterally produce prolonged I-blood levels. Salts of I and the following were prepared: PhCH2NPhCH2C(:NH)NH2, N-(2-dimethylaminopropyl)phenothiazine, 2-[(p-methoxybenzyl)(2-dimethylaminoethyl)amino]-pyridine, 2-(N-phenyl-N-benzylaminomethyl)-4,5-dihydroglyoxaline, and DL-1-[α-(p-chlorophenyl)benzyl]-4-methylpiperazine.

IT 882741-24-4, Nicotinamide, N,N-diethylthio-, penicillin G salt (preparation of)

RN 882741-24-4 CAPLUS

CN INDEX NAME NOT YET ASSIGNED

CM 1

CRN 882741-23-3 CMF C10 H14 N2 O S2

CM 2

CRN 881025-87-2 CMF C16 H18 N2 O4 S

Relative stereochemistry.

L10 ANSWER 65 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1953:62026 CAPLUS

DN 47:62026

OREF 47:10549e-f

TI Acylated sulfonamides

PA Badische Anilin- & Soda-Fabrik (I. G. Farbenindustrie Akt.-Ges. "In Auflosung")

DT Patent

LA Unavailable

FAN.CNT 1

PATENT NO. KIND DATE APPLICATION NO. DATE

PI GB 692651 19530610 GF

AB See Ger. 830,507 (C.A. 47, 6982g).

RN 113513-61-4 CAPLUS

L10 ANSWER 66 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1953:62025 CAPLUS

DN 47:62025

OREF 47:10549e

TI Removal of impurities from 1,4-dicyano-2-butene

PA E. I. Du Pont de Nemours & Co.

DT Patent

LA Unavailable

FAN.CNT 1

			-	
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
LAN. CIVI I				

PI GB 692827 19530617 GB

AB See U.S. 2,557,258 (C.A. 46, 1582i).

RN 113513-61-4 CAPLUS

L10 ANSWER 67 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1953:62024 CAPLUS

DN 47:62024

OREF 47:10549d-e

TI β , γ -Olefinic ethers of halohydrins

IN Morris, Rupert C.; Van Winkle, John L.

PA Shell Development Co.

DT Patent

LA Unavailable

FAN.CNT 1

PATENT NO. KIND DATE APPLICATION NO. DATE

PI US 2608587 19520826 US

AB Equimolar proportions of CH2:-CHCH2Cl and epichlorohydrin at 130-250° in the presence of a cuprous catalyst give high yields of CH2ClCH(OCH2CH:CH2)CH2Cl. It is essential that the reaction be conducted in a vessel, the inner surface of which is devoid of ferromagnetic ferrous alloys having a microstructure other than austenitic. Cf. preceding abstract

RN 113513-61-4 CAPLUS

$$\begin{array}{c|c} Me & O & O & N \\ & & & \\ & & \\ S-NH-C & \\ & & \\ O & \end{array}$$

L10 ANSWER 68 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN 1953:41393 CAPLUS AN 47:41393 DN OREF 47:6982f-i,6983a Acylated sulfonamides IN Krzikalla, Hans; Plankenhorn, Erwin Badische Anilin- & Soda-Fabrik (I. G. Farbenindustrie Akt.-Ges. "In PA Auflosung") DTPatent Unavailable T.A FAN.CNT 1 APPLICATION NO. PATENT NO. KIND DATE DATE -----____ PΙ DE 830507 19520204 DE 1950-B2060 19500214 AB Treating carboxylic acids with sulfonyl isocyanates at elevated temps. (100-200°) and possibly in the presence of a higher-boiling inert diluent gives, corresponding to RCO2H + OCNSO2R' → RCONH-SO2R' + CO2, N-Acylsulfonamides useful as textile auxiliary agents or intermediates in the manufacture of dyes and pharmaceuticals. Heating glacial AcOH 6 and p-MeC6H4SO2NCO (I) 20 at 130° until the gas evolution has ceased gives N-acetyl-p-toluenesulfonamide 15 parts by weight, m. 138° (from EtOH), acid number 260. Replacing I by an alkylsulfonyl isocyanate (prepared from an alkanesulfonylchloride from the sulfochlorination of a liquid paraffin hydrocarbon mixture with Cl and SO2) gives an oily N-acetylalkanesulfonamide. Similarly are prepared: N-benzoyl-p-toluenesulfonamide, m. 146° (from EtOH), acid number 197 (calculated 203), from I and BzOH; N-benzoylbenzenesulfonamide, m. 146°; N-phenylacetyl-p-toluenesulfonamide, m. 148-9°, acid number 191 (calculated 193), from I and PhCH2CO2H; N-stearoyl-ptoluenesulfonamide, m. 78° (from EtOH), acid number 132 (calculated 128), from I and stearic acid; N-oleoyl-p-toluenesulfonamide, m. 59° (from glacial AcOH), acid number 131 (calculated 129), from I and oleic acid; N,N'-bis(p-toluenesulfonyl)adipamide, m. 229° (from BuOH), acid number 243 (calculated 248), from I and adipic acid; N-(ptoluenesulfonyl)nicotinamide, m. 222° (from MeOH), acid number 209 (calculated 203) from I and nicotinic acid; N-(p-toluenesulfonyl)abietinamide, acid number 123, from I and abietic acid. IΤ 113513-61-4, Nicotinamide, N-p-tolylsulfonyl-(preparation of) 113513-61-4 CAPLUS RN CN 3-Pyridinecarboxamide, N-[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX

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L10 ANSWER 69 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
     1948:32159 CAPLUS
AN
     42:32159
DN
OREF 42:6851h-i,6852a-c
     N-Acyl-p-aminobenzenesulfonamides
PA
     J. R. Geigy, A.-G.
     Patent
DT
LA
     Unavailable
FAN.CNT 1
                     KIND
    PATENT NO.
                                         APPLICATION NO.
                               DATE
                                                                 DATE
                               ----
     GB 598472
                               19480219 GB 1944-21582
                                                                   19441103
PI
     Products having greater effectiveness against infective agents and low
AB
     toxicity are prepared by causing a p-aminobenzenesulfonamide to react with a
     carbonyl halide containing a heterocyclic residue or by condensing a
     heterocyclic acid amide with p-O2NC6H4SO2Cl, followed by reduction of the
     nitro group. Thus, O2NC6H4SO2NHNa (I) 44.8 suspended in PhNO2 150 is
     gradually mixed with 3,5-dimethyl-4-isoxazolecarbonyl chloride 31.9 parts,
     the mixture heated at 50-60^{\circ} 4 h., and the product (II) dissolved in
     2 N Na2CO3 solution, filtered from unchanged I, precipitated with 2 N HCl, and
     recrystd. from EtOH. In an Fe reducing kier, Fe chips 68, saturated NaCl
     solution 400, H2O 400, and 30% HCl 72 parts are thoroughly stirred together
     for 15 min. at 98°. While maintaining this temperature,
     N-(p-nitrophenylsulfonyl)-3,5-dimethyl-4-isoxazolecarboxamide (II) 65
     parts is introduced in small portions and the reaction is complete in 1 h.
     The solution is made alkaline with 2 N NaOH, filtered from the sludge, the
     filtrate is acidified with 30% HCl, and the precipitated N-(p-
     aminophenylsulfonyl) acid (III) filtered with suction and purified by
     dissolving in 2 N Na2CO3 solution, precipitating with 2 N HCl, and
crystallizing from EtOH.
     By using appropriate acids, the following compds. are prepared:
     N-(4-aminophenylsulfonyl)-2,6-dimethyl-4-chloro-3-pyridinecarboxamide;
     N-(4-semicarbazidophenylsulfonyl)-2,6-dimethyl-4-chloro-3-
     pyridinecarboxamide; the Na salt of N-[p-(sulfomethylamino)phenylsulfonyl]-
     4-chloro-2,6-dimethyl-3-pyridinecarboxamide; N-(4-aminophenylsulfonyl)-1-
     ethyl-2(1H)-pyridone-6-carboxamide; N-(4-aminophenylsulfonyl)-2,4-
     dimethylcoumalamide; N-(4-nitrophenylsulfonyl)-5-methyl-4-
     pyrimidinecarboxamide; N-(4-aminophenylsulfonyl)-2,6-dimethyl-4-ethoxy-3-
     pyridinecarboxamide; N-(4-aminophenylsulfonyl)-2,6-dimethyl-4-
     (methylmercapto)-3-pyridinecarboxamide; N-(4-nitrophenylsulfonyl)-5-tert-
     butylfuramide, m. 212° and its 4-amino analog, m. 239°,
     obtained by Fe + HCl reduction Cf. C.A. 41, 2440a; 42, 219b.
     845718-25-4, Nicotinamide, 4-chloro-2,6-dimethyl-N-sulfanilyl-
IT
     845745-75-7, Nicotinamide, 2,6-dimethyl-4-(methylthio)-N-
     sulfanilyl- 845752-18-3, Nicotinamide, 4-ethoxy-2,6-dimethyl-N-
     sulfanilyl- 845752-30-9, Nicotinamide, 1-ethyl-1,6-dihydro-6-oxo-
     N-sulfanilyl- 845960-89-6, Nicotinamide, 4-chloro-2,6-dimethyl-N-
     (N-sulfomethylsulfanilyl)-, sodium salt 845960-92-1,
     Nicotinamide, 4-chloro-2,6-dimethyl-N-(N-ureidosulfanilyl)-
     858480-20-3, Semicarbazide, 1-[p-[(4-chloro-2,6-
     dimethylnicotinoyl)sulfamoyl]phenyl]-
        (preparation of)
RN
     845718-25-4 CAPLUS
CN
     Nicotinamide, 4-chloro-2,6-dimethyl-N-sulfanilyl- (5CI) (CA INDEX NAME)
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RN 845745-75-7 CAPLUS

CN Nicotinamide, 2,6-dimethyl-4-(methylthio)-N-sulfanilyl- (5CI) (CA INDEX NAME)

RN 845752-18-3 CAPLUS

CN Nicotinamide, 4-ethoxy-2,6-dimethyl-N-sulfanilyl- (5CI) (CA INDEX NAME)

RN 845752-30-9 CAPLUS

CN Nicotinamide, 1-ethyl-1,6-dihydro-6-oxo-N-sulfanilyl- (5CI) (CA INDEX NAME)

RN 845960-89-6 CAPLUS

CN Nicotinamide, 4-chloro-2,6-dimethyl-N-(N-sulfomethylsulfanilyl)-, sodium salt (5CI) (CA INDEX NAME)

Na

RN 845960-92-1 CAPLUS

CN Nicotinamide, 4-chloro-2,6-dimethyl-N-(N-ureidosulfanilyl)- (5CI) (CA INDEX NAME)

RN 858480-20-3 CAPLUS

CN Semicarbazide, 1-[p-[(4-chloro-2,6-dimethylnicotinoyl)sulfamoyl]phenyl]-(5CI) (CA INDEX NAME)

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L10 ANSWER 70 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
AN
     1948:29905 CAPLUS
     42:29905
DN
OREF 42:6379d-h
     Acylsulfonamides
TI
     J. R. Geigy A.-G.
DT
     Patent
     Unavailable
LA
FAN.CNT 1
                                                                          DATE
     PATENT NO.
                           KIND
                                   DATE
                                                APPLICATION NO.
                                   19480220
     GB 598536
PI
     Compds. of the general formula R2R1CNSO2R, where R1 is aliphatic, aromatic,
AΒ
     aralkyl, cycloalkyl, or heterocyclic, R is a substituted or unsubstituted
     residue, and R2 is a substituted or unsubstituted amino or imido ester
     group, can be easily hydrolyzed to the corresponding acylsulfonamide of
     formula R1CONHSO2R. Thus, p-MeC(NH2):NSO2C6H4NO2 (I) 10 and 3.5% HCl 100
     parts are stirred at 90-100° 4 h. After cooling, the mass is made
     alkaline with NaOH, filtered, and acidulated, giving N-acetyl-4-
     nitrobenzenesulfonamide, m. 194°. From the corresponding amidines,
     the following compds. were obtained by similar procedure:
     N1-Acyl-p-nitrobenzenesulfonamides: isovaleryl, m. 144-5°;
      (\beta,\beta-dimethylacrylyl), m. 155°; (3,4-dimethylbenzoyl), m.
     192°; (3,4-dimethylhydrocinnamoyl), m. 85-6°; 1-naphthoyl, m. 198-200°; 2-furoyl, m. 208-10°. N1-Acylsulfanilamides:
     isovaleryl, m. 130°; butyryl, m. 126°; isobutyryl, m.
     199°; (\beta, \beta-dimethylacrylyl), m. 184-5°;
      (\alpha, \beta, \beta-trimethylacrylyl), m. 181-2°;
      (\alpha-propoxyproprionyl), m. 140°; (\alpha-propoxyisobutyryl),
     m. 135-6°; (\beta, \beta-dimethylacrylyl), m. 155°;
     (4-methylbenzoyl), m. 178-9°; (4-ethylbenzoyl), m. 162-3°; (4-propylbenzoyl), m. 162°, [4-(ethylmercapto)benzoyl], m.
     185°; (3,4-dimethylbenzoyl), m. 222°; (3-propyl-4-
     methoxybenzoyl), m. 213°; (3-allyl-4-methoxybenzoyl), m.
202-3°; 1-cyclopentenoyl, m. 202°; (1-cyclohexenylacetyl),
     m. 176-7°; (3,4-dimethylhydrocinnamoyl), m. 75-8°;
      (4-methylcinnamoyl), m. 209-10^{\circ}; (4-methoxy-\beta-
     methylcinnamoyl), m. 182-4°; hydrocinnamoyl, m. 160-1°;
      1-naphthoyl, m. 206-7°; (4-methyl-1-naphthoyl), m. 222°;
      2-naphthoyl, m. 205°; (1-methoxy-2-naphthoyl), m. 230°;
      (1-methyl-2-indenylcarbonyl), m. 233° (decomposition); 2-furoyl, m.
      188-9°; nicotinyl, m. 256-7°. Benzenesulfonamides:
      N-(4-chlorobenzoyl)-4-Me, m. 195°; N-(3,4-dimethylbenzoyl), m.
      140°; N-1-naphthoyl-2,3,5,6-tetramethyl, m. 220°;
      N-proprionyl-3,4-dichloro, m. 126°; N-stearoyl-3,4-dichloro. Other
      compds. formed are: N-1-naphthoyl-2-naphthalenesulfonamide,
      C10H7CONHSO2C10H7; N-(4-methylbenzoyl)-1-naphthalenesulfonamide,
      MeC6H4CONHSO2C10H7, m. 196°; and N-(3,4-dimethylbenzoyl)-2-
      naphthalenesu fonamide, 3,4-Me2C6H3CONHSO2C10H7 m. 210°. Cf. C.A.
      41, 2440g.
      6005-34-1, Nicotinamide, N-sulfanilyl-
ΙT
         (preparation of)
RN
      6005-34-1 CAPLUS
      Nicotinamide, N-sulfanilyl- (8CI) (CA INDEX NAME)
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L10 ANSWER 71 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
     1947:29342 CAPLUS
AN
     41:29342
DN
OREF 41:5898f-i,5899a
     N-Sulfanilyl carboxamides
IN
     Martin, Henry; Hafliger, Franz; Neracher, Otto
PA
     J. R. Geigy A.-G.
DT
     Patent
     Unavailable
LA
FAN.CNT 1
                                                                  DATE
                    KIND
                                DATE
                                          APPLICATION NO.
     PATENT NO.
     US 2417006
                                19470304 US 1944-533659
                                                                    19440501
PΙ
ΑB
     Hydrolysis of N'-sulfanilylamidines is a practical method of preparing acyl
     sulfanilamides. N-Sulfanilylisovaleramide, m. 130° (from dilute
     MeOH), is obtained by hydrolysis of 10 parts N'-sulfanilylisovaleramidine,
     m. 118-20°, with 10 parts of 3.5% HCl at 90-100° 2 hrs.,
     followed by neutralization with Na2CO3 and acidification with AcOH.
     Similarly N-sulfanilyl derivs. of the following amides were prepared:
     butyramide, m. 126° (amidine, m. 70-2°); isobutyramide, m.
     199°; β,β-dimethylacrylamide, m. 184-5° (amidine
     m. 128-9°); 4-methylbenzamide (I), m. 178-9° (cf. preceding
     abstract, m. 144°) (amidine, m. 236°); 4-ethylbenzamide (II), m. 162-3°; 4-propylbenzamide, m. 162°; 4-
     (ethylmercapto) benzamide (III), m. 185°; 3,4-dimethylbenzamide
     (IV), m. 222° (amidine, m. 218-20°); 3-propyl-4-
     methoxybenzamide, m. 213°; 3-allyl-4-methoxybenzamide, m.
     202-3°; 1-cyclopentene-1-carboxamide, m. 202°;
     1-cyclohexene-1-acetamide, m. 176-7°. IV is also obtained by a
     24-hr. hydrolysis of the following derivs. of N'-sulfanilyl-3,4-
     dimethylbenzamidine: N,N-diethyl-, m. 148-50°; N-phenyl-, m.
     198-200°; N,N-dimethyl-; N-tolyl-; and by a 12-hr. hydrolysis of Et
     N-sulfanily1-3,4-dimethylbenzimidate, m. 328-9° (decomposition). I and
     II are also obtained from the corresponding benzimidic acid esters. A
     4-hr. hydrolysis of the proper amidines yields N-sulfanilyl derivs. of the
     following amides: 3,4-dimethylhydrocinnamamide, m. 76-8°;
     p-methylcinnamamide, m. 209-10°; p-methoxy-\alpha-
     methylcinnamamide, m. 182-4°; hydrocinnamamide, m. 160-1°;
     1-naphthamide; 4-methyl-1-naphthamide, m. 222°; 2-naphthamide;
     1-methoxy-2-naphthamide, m. 230°; 1-methyl-2-indenecarboxamide, m.
     233°. A 3-hr. hydrolysis of the proper amidines yields
     N-sulfanilyl derivs. of 2-furamide, m. 188-9° (cf. preceding
     abstract, m. 191-2°) (amidine, m. 165-6°), and nicotinamide,
     m. 256-7°.
     6005-34-1, Nicotinamide, N-sulfanilyl-
IT
        (preparation of)
RN
     6005-34-1 CAPLUS
     Nicotinamide, N-sulfanilyl- (8CI) (CA INDEX NAME)
CN
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$$\begin{array}{c|c} H_2N & O & O & N \\ \parallel & \parallel & \parallel & \parallel \\ S-NH-C & & \parallel & \parallel \\ O & & & O & N \\ \end{array}$$

L10 ANSWER 72 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

AN

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1947:29228 CAPLUS
     41:29228
DN
OREF 41:5864e-i,5865a-c
     Certain sulfanilamide derivatives of nicotinic acid
ΑIJ
     Sadykov, A. S.; Maksimov, V. I.
     Middle-Asiatic State Univ.
CS
     Zhurnal Obshchei Khimii (1946), 16, 1719-28
SO
     CODEN: ZOKHA4; ISSN: 0044-460X
     Journal
DT
     Unavailable
LΑ
     In view of the partial control of the toxic effects of sulfa drugs by
AΒ
     administration of nicotinic acid, several derivs. of sulfa drugs containing a
     nicotinic acid residue were prepared Sulfanilamide (7.2 g.) in 30 cc.
     pyridine bases (crude) was treated with 7 g. nicotinyl chloride (I) and
     the mixture was heated on a steam bath 2 h.; after removal of the solvent in
     vacuo and dilution with H2O, the crude product was purified by crystallization
from
     50% EtOH, then from EtOH, to yield. N1-nicotinylsulfanilamide, m.
     256-7° (84.6%), identical with the Crossley, et al., product (C.A.
     34, 392.8). I (28.8 g.) in 100 cc. pyridine bases was treated with 42 g.
     p-AcNHC6H4SO2NH2 and heated on a steam bath for 3 h.; after dilution with
     water, 45 g. N1-nicotinyl-N4-acetylsulfanilamide, m. 213-15° (from
     50% EtOH) (methiodide, m. 196-7° (from EtOH)) was obtained; the Ac
     group is readily removed by hydrolysis with 15% HCl at 50-60° 3 h.
     I (14.1 g.) in 30 cc. pyridine bases was treated with 9.4 g.
     2-aminopyridine and the mixture was heated on a steam bath for 3 h.; after
     removal of the solvent in vacuo 20 g. 2-nicotinylaminopyridine, m.
     230° (from EtOH) (picrate, m. 220-1° (from EtOH);
     methiodide, m. 192-3° (from EtOH)) was obtained. I (7.2 g.) in 25
     cc. pyridine bases and 12 g. sulfapyridine heated on a steam bath 3 h.
     yielded after dilution with water 12 g. N4-nicotinyl-N1-(2-
     aminopyridyl)sulfanilamide (nicotinylsulfapyridine), m. 185-6°
      (from EtOH); picrate m. 149-50° (from EtOH); methiodide m.
     228-9° (from EtOH). I (14.2 g.) in 50 cc. pyridine bases and 10.8
     g. sulfaquanidine heated on a steam bath 2 h. yielded
     dinicotinylsulfaguanidine, m. 219-20° (from 50% EtOH), in 12-g. yield; picrate m. 191-2° (from EtOH); similar reaction, using N4-acetylsulfaguanidine, gave 12 g. nicotinyl derivative (from 7.2 g. I), m. 258-9° (from 50% EtOH); picrate m. 200-2° (from EtOH).
     Similar reaction of sulfa-4-methylthiazole gave the N4-nicotinyl derivative
      (15 g. from 7.2 g. I), m. 230-2^{\circ}. Nicotinic acid (12.3 g.), 12.1
     g. PhNEtH, and 10 g. PCl5 were heated to 200-10° 4 h.; on cooling,
     diluting with 200 cc. H2O, and making alkaline with 50% NaOH there was obtained
     N-phenyl-N-ethylnicotinamide, b3 186-90°, m. 63° (from
     Me2CO); picrate m. 154-5^{\circ} (from EtOH); methiodide m.
     137-7.5° (from EtOH). PhNHEt (121 g.) treated, with cooling, with
     78.5 g. AcCl gave 150 g. N-Ac derivative, m. 53°, which was treated at
     20-5^{\circ} with 350 cc. ClSO3H; the mixture was heated to 60-70^{\circ} 3
     h., poured on ice, and filtered to yield 200 g. p-(N-
     ethylacetamido) benzenesulfonyl chloride, m. 139-40° (from
      (CH2Cl)2); this was added slowly to 380 g. concentrated NH4OH to yield 150 g.
     p-(N-ethylacetamido)benzenesulfonamide, m. 123-4° (from water).
     The latter (50 g.) in 150 cc. 20% HCl was heated to 65-70^{\circ} for 3
     h., to yield on cooling and neutralization with Na2CO3,
     N4-ethylsulfanilamide, m. 110-1^{\circ}. When this (5 g.) and 3.6 g. I were heated on a steam bath 4 h. in 20 cc. pyridine bases there was
     obtained, after the removal of the solvent in vacuo, 5.6 g.
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N1-nicotinyl-N4-ethylsulfanilamide, m. 229-30° (from 70% EtOH); picrate m. 218° (from EtOH); methiodide m. 214-15° (decomposition; from EtOH); the preparation was confirmed by a similar condensation

of I with the N4-acetyl-N4-Et derivative to yield N1-nicotinyl-N4-ethyl-N4-acetylsulfanilamide, m. 242-3 $^{\circ}$ (from EtOH), which on hydrolysis with 20 $^{\circ}$ HCl for 5 h. at 65-70 $^{\circ}$ gave a product identical with that of direct condensation.

IT 6005-34-1, Nicotinamide, N-sulfanilyl- 845754-75-8,
Nicotinamide, N-(N-ethylsulfanilyl)- 845754-82-7, Nicotinamide,
N-(N-ethylsulfanilyl)-, methiodide 845754-83-8, Nicotinamide,
N-(N-ethylsulfanilyl)-, picrate 845960-04-5, Nicotinamide,
N-(N-acetyl-N-ethylsulfanilyl)- 845960-39-6, Nicotinamide,
N-(N-acetylsulfanilyl)- 845960-40-9, Nicotinamide,

N-(N-acetylsulfanilyl)-, methiodide 860402-80-8, Nicotinanilide, 4'-(nicotinoylamidinosulfamoyl)- 860430-81-5, Sulfanilamide, N4-ethyl-N1-nicotinoyl-, picrate 860430-83-7, Sulfanilamide,

N4-ethyl-N1-nicotinoyl-, methiodide

(preparation of)

RN 6005-34-1 CAPLUS

CN Nicotinamide, N-sulfanilyl- (8CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & & & \\ & & & \\ &$$

RN 845754-75-8 CAPLUS

CN Nicotinamide, N-(N-ethylsulfanilyl)- (5CI) (CA INDEX NAME)

RN 845754-82-7 CAPLUS

CN Nicotinamide, N-(N-ethylsulfanilyl)-, methiodide (5CI) (CA INDEX NAME)

CM 1

CRN 845754-75-8 CMF C14 H15 N3 O3 S

CM 2

CRN 74-88-4 CMF C H3 I

 H_3C-I

RN 845754-83-8 CAPLUS

CN Nicotinamide, N-(N-ethylsulfanilyl)-, picrate (5CI) (CA INDEX NAME)

CM 1

CRN 845754-75-8 CMF C14 H15 N3 O3 S

CM 2

CRN 88-89-1 CMF C6 H3 N3 O7

RN 845960-04-5 CAPLUS

CN Nicotinamide, N-(N-acetyl-N-ethylsulfanilyl)- (5CI) (CA INDEX NAME)

RN 845960-39-6 CAPLUS

CN Nicotinamide, N-(N-acetylsulfanilyl)- (5CI) (CA INDEX NAME)

RN 845960-40-9 CAPLUS

CN Nicotinamide, N-(N-acetylsulfanilyl)-, methiodide (5CI) (CA INDEX NAME)

CM 1

CRN 845960-39-6 CMF C14 H13 N3 O4 S

CM 2

CRN 74-88-4 CMF C H3 I

H3C-I

RN 860402-80-8 CAPLUS

CN Nicotinanilide, 4'-(nicotinoylamidinosulfamoyl)- (5CI) (CA INDEX NAME)

RN 860430-81-5 CAPLUS

CN Sulfanilamide, N4-ethyl-N1-nicotinoyl-, picrate (5CI) (CA INDEX NAME)

CM 1

CRN 845754-75-8 CMF C14 H15 N3 O3 S

CM 2

CRN 88-89-1 CMF C6 H3 N3 O7

RN 860430-83-7 CAPLUS

CN Sulfanilamide, N4-ethyl-N1-nicotinoyl-, methiodide (5CI) (CA INDEX NAME)

• 1-

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L10 ANSWER 73 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
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AN 1947:24017 CAPLUS

DN 41:24017

OREF 41:4809a-i,4810a-i,4811a

TI Valuable derivatives of sulfonamides

IN Dohrn, Max; Diedrich, Paul

PA Schering Corp.

DT Patent

LA Unavailable

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 2411495		19461119	US 1939-253734	19390131

AB Sulfonamide derivs. acylated at the sulfonamide N, of the general formula RSO2NHX, in which R stands for an aromatic, heterocyclic, or mixed residue and X for an acyl radical, are described. In these compds. the H atom can be replaced by metals, the resulting salts being easily soluble in water with neutral reaction. The new compds. are made either by direct acylation of the sulfa drugs and partial saponification of the diacyl derivs. or by reacting sulfonyl chlorides or anhydrides with acyl amides. Another method consists in acylating nitro- or halo-substituted sulfonamides and then substituting the nitro or halogen groups by the NH2 group. The alkali or alkaline earth salts of the new compds. are prepared by simply adding the calculated

made from their sulfates and the Ba salt of the new compds. Organic bases can also be used for salt formation. The products have the same therapeutic use as the parent sulfa compds. p-RNHC6H4SO2NHX; Number, R, X, M.p.; I, Ac, Ac, 253° (d.); II, H, Ac, 181°; III, EtCO, COEt, 232°; IV, H, COEt, 130-1°; V, Ac, Bz, 245-6° (d.); VI, H, Bz, 179-86°; VII, PhCH2, Ac, 143-4°; VIII, p-AcNHC6H4SO2, Ac, 178°; IX, p-H2NC6H4SO2, Ac, 187°; X, H, C6H4SO2NH2(m), 156°; XI, Ac, C6H4SO2NHAc(m), 145-6°; XII, PhCH2OCO, H, 192-2.5°; XIII, PhCH2OCO, Ac, 167-8°; XIV, EtoCo, H, 238°; XV, EtoCo, Ac, 244°; XVI, MeOCo, H, 226-7°; XVII, glucoside, Ac, 191°; XVIII, H, nicotinoyl, 246°; XIX, EtoCo, nicotinoyl, 241°; XX, EtoCo, COPr, 217-18°; XXI, H, COPr, 125°; XXII, EtOCO, COCH:CHMe, 224°; XXIII, H, COCH: CHMe, 175°; XXIV, Ac, COC6H4NO2(p), 256°; XXV, EtoCo, COEt, 208°; XXVI, EtoCo, COCH2Ph, 209°; XXVII, H, COCH2Ph, 182°; XXVIII, EtoCo, COCH2Cl, 229°; XXIX, EtOCO, COCH2NH2, 223°; XXX, EtOCO, COC6H4OH(o), 242°; XXXI, H, COC6H4OH(o), 200-1°; XXXII, EtOCO, COC.O.CH, 259° (d.); XXXIII, H, COC.O.CH, 188-9°; XXXIV, H, CH-CH hydnochauloyl (chaulmoogroyl), 131°; XXXV, EtOCO, CO2Et, 162°; XXXVI, H, CO2Et, 133°; XXXVII, AcNH, Ac, 278-9°; XXXVIII, H2N, Ac; XXXIX, PhNH, H, 178°; I, prepared from sulfanilamide and Ac2O, prisms from alc., insol. in water, soluble in alkalies, forms neutral salts. When it is refluxed in a quantity of 2 N NaOH insufficient for complete saponification, then acidified, and the precipitate is

treated with dilute Na2CO3 solution, II dissolves and the p-AcNHC6H4SO2NH2 formed simultaneously remains undissolved; II, colorless crystals, is easily soluble in alc. and acetone, difficultly in water, insol. in benzene and CHCl3. V is prepared from p-AcNHC6H4SO2NH2 and BzCl in NaOH. X, from p-AcNHC6H4SO2Cl and m-H2NC6H4, followed by saponification, gives XI with Ac2O. XII is obtained in 250-g. yield by adding 340 g. ClCO2CH2Ph to 172 g.

sulfanilamide at 0° with stirring, separating the XII after several hrs., washing it with dilute HCl, and crystallizing it from MeOH; boiled with 5 times its weight of Ac2O it gives XIII, 200 g. of which, shaken in 3 l. alc. with 5 g. Pd black and H, yields 106 g. II. XIV, from NH3 and an ether solution of N-carbethoxysulfanilyl chloride (m. 104-5°, prepared from PhNHCO2Et and ClSO3H at 0° and then at 55-60°, precipitated in ice water, and purified from MeOH and water). XV, from XIV and Ac2O, gives II when heated 10 min. at 80° with 7 times its weight of 2 N NaOH. N-Carbomethoxysulfanilyl chloride, from p-MeO2CNHC6H4SO3Na and PCl5, m. 117-18°. XVII, from II and glucose refluxed in EtOH, needles from absolute EtOH, easily soluble in water; its alkali salts dissolve easily in water

with neutral reaction. XIX, from XIV and nicotinoyl chloride in pyridine, saponified by 2 N NaOH 24 h. at room temperature to XVIII. XX, from XIV and Prcocl, saponified to XXI by 2 N NaOH at room temperature XXII is prepared by heating 24.5 g. XIV, 125 g. MeCH: CHCO2H, and 11 g. MeCH: CHCOCl 2 h. to 145°, decomposing with ice water, dissolving the precipitate in Na2CO3, and precipitating with AcOH. XXVI, from XIV heated several hrs. at 160-70° with PhCH2COCl. XXVIII, from XIV and (ClCH2CO)2O heated 1 h. at 120-5°, gives XXIX with concentrated NH3 solution at room temperature XXX, from XIV and o-HOC6H4COCl heated several hrs. at 170-80°, saponified to XXXI by 2 N NaOH. XXXII, from XIV and pyromucyl chloride in C5H5N with cooling, saponified to XXIII by 2 N NaOH. XXXIV, prepared by heating XIV with hydnochauloyl chloride at 148°, precipitating in water, and repptg. from Na2CO3 solution XXXV, from XIV and ClCO2Et in C5H5N, from sulfanilamide and 2 mols. C1CO2Et, or from p-EtO2CNHC6H4SO2Cl heated with urethane at 140-50° until a sample is readily soluble in dilute Na2CO3 solution 2-Acetamido-5-(acetylsulfamyl)pyridine (XXXVII), from 2-chloro-5pyridinesulfonamide reacted with concentrated NH4OH in a closed container at 150° and the product boiled with Ac20 and recrystd. from water. Other compds. mentioned are: 4-(Acetylsulfamyl)-2',4'-diaminoazobenzene (XL), prepared from diazotized II and m-C6H4(NH2)2, is precipitated by AcOH

hot Na2CO3 solution in blue-red lustrous leaflets, decomposing 180°. 1,3-Bis[4-(acetylsulfamyl)phenyl]urea, prepared from II in NaOH at 50° with phosgene and purified by precipitating with AcOH from hot Na2CO3 solution, needles, decompose 255°, very difficultly soluble in water. 1-[4-(Acetylsulfamyl)phenylazo]-2-naphthol-6,8-disulfonic acid, from diazotized II and 2,6,8-C10H5(OH) (SO3Na)2 in Na2CO3 solution; after acidifying slightly the Na salt is precipitated by saturating with NaCl and recrystd.

from dilute alc. in vermilion reddish prismatic needles, decompose 333°. N,N'-Bis(N-carbethoxysulfanilyl)adipamide, from XIV and adipyl chloride at 150°, crystals from dilute alc., m. 220° (decomposition), saponified to the 4,4'-diamino compound, m. 212° (from dilute alc.). N,N'-Bis(N-carbethoxysulfanilyl)mucic acid amide, from XIV and mucic acid chloride at 190°, m. 201°, saponified by 2 N NaOH to the 4,4'-diamino compound, m. 233°. 1-[4-(Acetylsulfamyl)phenylazo]-2,6-diaminopyridine, from diazotized II and 2,6-diaminopyridine in acid solution after addition of NaOAc, orange reddish needles from alc., m. 191-2°, soluble in Na2CO3 solution Salts of II: Na, from 21.4 g. II dissolved in 100 mL. N NaOH, concentrated, precipitated with EtOH, and recrystd. from

dilute alc., m. 257°; Ba, m. 185° (decomposition), from dilute alc.; Cu, from the Ba salt with CuSO4, greenish powder; NH4, m. 156° (decomposition); pyridine, from II dissolved in hot C5H5N, cooled, and the precipitate

recrystd. from alc., m. 120°; diethanolamine, m. (about)

155°; Ca, from II and CaCO3; Ag, precipitated from II in water with AgNO3, washed with water, alc., and ether, and dried, m. 216°; Hg, from II in water with Hg(OAc)2, m. 251° (decomposition); quinine, from 31.4 g. II and 32.4 g. quinine in alc. and evaporation of the latter, soluble in water, m.

73°; morphine, from the components in alc., with heating, precipitated by addition of ether, m. about 160°. Ca salt of IV, from IV and CaCO3 in water, crystals from dilute alc., decompose 283°. Mg salt of XXXIII, from XXXIII and MgCO3 in boiling water, crystals from dilute alc. Na salt of XVIII, from dilute alc., decompose above 270°. Mg salt of XVII, from XVII and MgCO3 in boiling water, m. 165-7°. Na salt of IX, from IX with dilute NaOH and precipitation with alc. Ca salt of VII, from VII

 $\mbox{{\it CaCO3}}$ by boiling several hrs. in water and precipitating from the concentrated solution

with alc., m. 268° (decomposition). Na salt of XL, orange-brown needles from water with alc. and ether, decompose 207°.

IT 6005-34-1, Nicotinamide, N-sulfanilyl-845674-82-0, Nicotinamide, N-(N-carboxysulfanilyl)-, ethyl ester (preparation of)

RN 6005-34-1 CAPLUS

and

CN Nicotinamide, N-sulfanilyl- (8CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & & \\ & & & & \\ & & \\ & & & \\ & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & &$$

RN 845674-82-0 CAPLUS

CN Nicotinamide, N-(N-carboxysulfanilyl)-, ethyl ester (5CI) (CA INDEX NAME)

- L10 ANSWER 74 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
- AN 1947:2208 CAPLUS
- DN 41:2208
- OREF 41:409h-i,410a-i,411a-b
- TI Amidines. II. Preparation of cyanides, amides, and amidines from carboxylic acids
- AU Oxley, P.; Partridge, M. W.; Robson, T. D.; Short, W. F.
- CS Boots Pure Drug Co. Ltd., Nottingham, UK
- SO Journal of the Chemical Society (1946) 763-71 CODEN: JCSOA9; ISSN: 0368-1769
- DT Journal
- LA Unavailable
- OS CASREACT 41:2208
- cf. C.A. 40, 4367.1. It is suggested that the reaction between RCO2H and AΒ R'SO2NH2 can be represented as occurring in 5 stages: (A) RCO2H + R'SO2NH2 RCONH2 + R'SO3H; (B) RCONH2 + R'SO2NH2 + R'SO3H → RCONHSO2R' + R'SO3NH4; (C) RCONHSO2R' RC(:NH)OSO2R'; (D) RC(:NH)OSO2R' → RCN + R'SO3H; (E) RCN + R'SO3NH4 \rightarrow RC(:NH)NH2.R'SO3H. BzOH and PhSO2NMe2, heated at 235-40°, react exothermically to yield 83% BzNMe2 and PhSO3H. The constituents in hot Me2CO yield nicotinic acid benzenesulfonate (I), m. 160°. I and PhSO2NEt2 at 220° for 1 h. give 81% nicotinodiethylamide (II). More direct evidence for the functional exchange is provided by the fact that the reaction between RCO2H and RSO2NH2 can be arrested at this stage. Nicotinic acid (12.3 g.) and 31.4 g. PhSO2NH2, kept at 225° for 4.5 h., give 9 g. PhSO2NH2 and 17.5 g. nicotinamide benzenesulfonate, m. 157°; this results also from the components in Me2CO. On the other hand, I and PhSO2NH2, heated at 230° for 40 min., yield 75% 3-cyanopyridine benzenesulfonate, m. 132°. When the RCO2H contains no basic group, the reaction can be arrested at stage A by the addition of a base. Thus, 1mol each of p-HO2CC6H4SO2Me, PhSO2NH2, and C5H5N give 33.4% (95% on acid consumed) p-carbamylphenyl Me sulfone (III), H2NCOC6H4SO2Me, m. 226-6.5°, when refluxed 3.25 h. C5H5N or quinoline almost completely inhibits the reaction between BzOH and PhSO2NH2 at 230-50°. The RCO2H-R'SO2NH2 exchange appears to be catalyzed by acids; thus, a small quantity of a sulfonic acid eliminates the period of induction sometimes observed in this reaction and shortens the duration of the first weakly exothermic phase in the reaction of PhSO2NH2 and p-O2NC6H4COCl; when heated at 145-50° for 5 h., these compds. give 60% N-p-nitrobenzoylbenzenesulfonamide (IV), m. 216-17°; IV results also from PhSO2NH2 and p-O2NC6H4CO2H on heating at 220°, the reaction being accelerated by the addition of a small quantity of PhSO3H.H2O; the temperature changes which occur during the reaction are shown in curves;

the

temperature rise is much greater with the catalyst. IV, heated at 220° 40 min., gives 81% p-O2NC6H4CN (66% after heating 18 min.). The o-NO2 isomer of IV, m. 171° (46% on basis of acid or 64% on basis of amide); heated at 225° for 8 min., it yields 42% o-O2NC6H4CN. p-HO2CC6H4SO2Me and PhSONH2, heated at 225° 70 min., give 62% p-NCC6H4SO2Me (V) and 20.5% N-(p-methylsulfonylbenzoyl)benzenesulfonamide (VI), m. 214.6-15°. If a small quantity of anhydrous PhSO3H is added, the yields are 80.3 and 1.2%, resp. p-ClOCC6H4SO2Me and PhSO2NH2, heated at 145° for 3.5 h., give 50.8% VI. An equimol. mixture of III, PhSO2NH2, and PhSO3H, heated at 198° 0.5 h., gives 81% V and 8% VI. When heated at 230° 1 h., VI gives 95% V. p-HO2CC6H4SO2Et and PhSO2NH2, heated at 225° 30 min., give 79% PhSO3NH4, 59% p-NCC6H4SO2Et, and 12.7% of the Et homolog of VI, m. 189°. Thus, it seems clear that "mixed imides" of the type of IV and VI are the

precursors of the cyanides produced from RCO2H and R'SO2NH2. The 2 exothermic phases involved in the preparation of p-O2NC6H4CN represent the acid-amide exchange (phase A) and the decomposition of the mixed amide (phases C and D). BzNHO2SPh results in 3% yield on heating BzNH2, PhSO2NH2, and PhSO3H at 155° for 3 h. PhSO2NHBz, heated at 200°, gives 89% PhCN and 82% PhSO3H. This establishes reaction D and the isomerization postulated in C is analogous to that which occurs in the Beckmann transformation of oximes. Stage E has been discussed in Part I. Details are given of the preparation of o- and p-HO2CC6H4SO2Me, p-O2NC6H4SO2Me, p-H2NC6H4SO2Me, p-NCC6H4SO2Me, and p-H02CC6H4SO2Et. p-MeC6H4SO2Pr (116 g.) in 600 cc. H2O at 90°, treated 12 h. with 185 g. KMnO4, give 47% p-carboxyphenyl Pr sulfone, m. 191-3°. p-MeC6H4SO2Na and p-O2NC6H4COCl in EtOH, boiled 1 h., give 56.5% p-tolyl p-nitrobenzyl sulfone, m. $185-9^{\circ}$; oxidation with Na2Cr2O7 in boiling AcOH gives 68% of p-carboxyphenyl p-nitrobenzyl sulfone, m. 295-300°. Examples are given of the preparation of 19 cyanides from an acid and a PhSO2NH2; 2-cyanophenyl Me sulfone, 83.5%, m. 103-4°; 4-cyanodiphenyl sulfone, 74%, m. 118°; 4-cyanophenyl 4-nitrobenzyl sulfone, 38%, m. 168-9°. The method fails with acids which are readily decarboxylated (e.g., p-HOC6H4CO2H) and much decarboxylation occurs with p-MeOC6H4CO2H, the yield of p-MeOC6H4CN being only 10%. It is convenient to employ PhSO2NH2 and p-MeOC6H4SO2NH2 because of their accessibility, although a somewhat lower yield (5%) of cyanide is usually obtained with the latter. There is usually no difficulty in regulating the exptl. conditions so that very little amidine is formed when a cyanide is the desired product of the reaction. Several examples are given in which an increased yield of amidine salt is obtained if the sulfonic acid is neutralized with dry NH3 before raising the temperature to accelerate the reaction of phase E. p-NCC6H4SO2Et (23 g.) and 25 g. PhSO3NH4, stirred at 245° for 4 h., give 52.5% p-amidinophenyl Et sulfone benzenesulfonate, m. 240°. p-Nitrobenzamidine picrate m. 240°. 3,4-Dichlorobenzamidine m. 94-5°; HCl salt m. 239.5°; benzenesulfonate m. 240-1°. Benzamide benzenesulfonate m. 121.5-2°.

RN 113513-72-7 CAPLUS

L10 ANSWER 75 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1946:24053 CAPLUS

DN 40:24053

OREF 40:4747b-g

TI Sulfonic acid amides of organic sulfonic acids and primary or secondary amines or amides

PA Aktieselskabet Grindstedvaerket

DT Patent

LA Unavailable

FAN.CNT 1

PATENT NO. KIND DATE APPLICATION NO. DATE

PI DK 63458 19450507 DK

AB A primary or secondary amine or amide is condensed with an aldehyde, and the product treated with the halide or anhydride of the desired sulfonic acid. Water is then added and, if necessary, a substance capable of splitting off H halide. The reaction proceeds as follows - R1NH2 →R2CHO R1N:CHR2 →R3SO2X R3SO2R1N-CHXR2 →H2O R1NH.S02R3 The aldehyde is regenerated in the last step of the process. Examples are given of the first intermediate compound by interaction of (1) BzH and AcNH2, (2) 2-hydroxynaphthaldehyde and 4-nitroaniline, (3) BzH and 5-amino-2-cyanothiazole and 5-amino-2-thiazolethiocarboxamide, (4) BzH and 5-amino-6-quinolinecarboxylic acid, (5) BzH and 4-aminomorpholine, (6) AcH and anthranilic acid, (7) PhCH:CHCHO and anthranilic acid, and (8) BzH and 4-amino-1,2,4-triazole. Specific examples are given of the preparation of (1) p-tolylsulfonamidobenzene from PhCH:NPh and p-MeC6H4SO2Cl, (2) p-acetamidophenylsulfonamidobenzene from PhCH:NPh and p-AcNHC6H4SO2Cl (I), (3) p-acetamidophenylsulfonamidothiazole from 2-salicylideneaminothiazole and I, (4) p-acetamidophenylsulfonamidopyridine from 2salicylideneaminopyridine and p-H2NC6H4SO2Cl, (5) Nmethylbenzenesulfonamide from PhCH:NMe and PhSO2Cl, (6) N-(p-acetamidophenylsulfonyl)anthranilic acid from N-ethylideneanthranilic acid and I, (7) phenylsulfonamidothiazole from N,N'-benzylidenebis(2aminothiazole) (II) and benzenesulfonic anhydride, (8) N-methyl-2-naphthalenesulfonamide from PhCH:NMe and 2-C10H7SO2Cl, (9) 2-(2-naphthylsulfonamido)thiazole from II and 2-naphthalenesulfonic anhydride, and (10) a sulfonamide from 4-benzylideneamino-1,2,4-triazole and p-MeC6H4SO2Cl. The preparation of N1,N4-diacetylsulfanilamide and, N4-acetyl-N1-nicotinylsulfanilamide (III) by similar methods is also described. N1-Nicotinylsulfanilamide may be obtained by the saponification of

IT 6005-34-1, Nicotinamide, N-sulfanilyl-(preparation of)

RN 6005-34-1 CAPLUS

CN Nicotinamide, N-sulfanilyl- (8CI) (CA INDEX NAME)

L10 ANSWER 76 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1945:27380 CAPLUS

DN 39:27380

OREF 39:4398b-d

TI Effects of sulfonamides on chick-brain tissue cultivated in vitro

AU deC. Saunders, John B.; Haymaker, Webb

SO Proceedings of the Society for Experimental Biology and Medicine (1945), 59, 306-9

CODEN: PSEBAA; ISSN: 0037-9727

DT Journal

LA Unavailable

AB Brain of 8-day-old chick embryos was cultivated in vitro in plasma to which sulfonamides were added in various concns. Cultures containing sulfadiazine and succinylsulfathiazole grew better than the controls at all concns. tested, even up to 5 times the saturation concentration Sulfapyrazine,

sulfapyridine, and sulfaguanidine in concns. up to saturation had no significant influence on growth. Sulfathiazole, sulfanilamide, succinylsulfanilamide, and nicotinylsulfanilamide were more or less toxic. The solubilities of the different sulfonamides in plasma, their effect on the pH of the plasma, and the influence of pH on brain-tissue growth were determined

IT 6005-34-1, Nicotinamide, N-sulfanilyl-

(effect on brain)

RN 6005-34-1 CAPLUS

CN Nicotinamide, N-sulfanilyl- (8CI) (CA INDEX NAME)

L10 ANSWER 77 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1945:16764 CAPLUS

DN 39:16764

OREF 39:2624e-f

TI N-Sulfanilylnicotinamide

IN Rosicky, Johann

DT Patent

LA Unavailable

FAN.CNT 1

PATENT NO. KIND DATE APPLICATION NO. DATE

PI DE 741685 19430930 DE

AB This compound is prepared from sulfanilamide or benzenesulfonamide substituted in the p-position by a group that can be transformed into a free amino group. The starting compound is made to react with quinolinic acid anhydride. The condensation is carried out either by fusing the two or by heating them in a solvent capable of withstanding a high temperature Either simultaneously with the condensation reaction or by subsequent treatment the product is decarboxylated.

IT 6005-34-1, Nicotinamide, N-sulfanilyl-

(preparation of)

RN 6005-34-1 CAPLUS

CN Nicotinamide, N-sulfanilyl- (8CI) (CA INDEX NAME)

$$\begin{array}{c|c} H_2N & O & O & N \\ \parallel & \parallel & \parallel & \parallel \\ S-NH-C & & \parallel & \parallel \\ O & & & & \\ \end{array}$$

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L10 ANSWER 78 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
    1945:11165 CAPLUS
AN
     39:11165
DN
OREF 39:1737d-g,1738a-b
     Sulfonamide derivatives of diaminodiphenyl sulfones
IN
     Tullar, Benjamin F.
     Parke, Davis & Co.
PA
DT
    Patent
LΑ
    Unavailable
FAN.CNT 1
    LALENT NO. KIND DATE
                               DATE APPLICATION NO.
                                           DATE
    US 2358365
                                19440919 US 1940-351151
                                                                   19400803
PΙ
AB
    The new compds. valuable as therapeutics, e.g., internal antiseptics, and
     intermediates for therapeutics have the general formula
     5-R3HN-2(p-R2HNC6H4SO2)C6H3SO2NR1R, where R2 and R3 represent members of
     the group consisting of H and organic carboxylic acid radicals, R1 is a
     member of the class consisting of H and organic carboxylic acid radicals and
     R is a member of the class H and an alkali metal. The compds. of the
     invention may be obtained by more than one method. For example, the
     corresponding sulfonamide substituted diphenyl sulfone having a nitro
     group substituted in one of the phenyl nuclei can first be prepared and the
     nitro group reduced to an amino group. Alternatively, the corresponding
     dinitrodiphenyl sulfide having a sulfonic acid group attached to the
     2-position of one of the phenyl nuclei can be reduced to the diamino
     sulfide and the sulfide oxidized to sulfone with or without protection of
     the amino groups by organic carboxylic acid. The resulting 2-sulfonic acid
     sulfone derivative can then be converted to the corresponding 2-sulfonamide
     compound The preparation of 4,4'-diaminodiphenyl-sulfone-2-sulfonamide, m.
     236°; 4,4'-diacetamido-diphenyl-sulfone-2-sulfonamide, m.
     275°; 4,4'-diacetamidodiphenyl-sulfone-2-N-acetylsulfonamide, m.
     approx. 295°; 4,4'-diaminodiphenyl-sulfone-2-N-acetylsulfonamide,
     m. approx. 285°; 4,4'-diacetamidodiphenyl-sulfone-2-N-nicotinyl-
     sulfonamide and the corresponding 4,4'-diamino compound, m. 245-50°
     is described. U.S. 2,358,366. 2-(4,4'-Diaminodiphenylsulfone-2-sulfonamido) pyridine, m. 2.15^{\circ} is prepared by oxidizing
     4,4'-dinitrodiphenyl-sulfide-2-sulfonic acid Na salt to the Na salt of
     4,4'-dinitrodiphenyl-sulfone-2-sulfonic acid, converting the latter by
     means of PC15 into 4,4'-dinitrodiphenyl-sulfone-2-sulfonyl chloride,
     treating the sulfonyl chloride with 2-aminopyridine to obtain
     2-(4,4'-dinitrodiphenyl-sulfone-2-sulfonamido)pyridine and reducing the
     nitro groups of the latter with production of \alpha-(4,4'-
     diaminodiphenyl-sulfone-2-sulfonamido)pyridine (2-(5-amino-2-
     sulfanilylphenylsulfonamido)pyridine).
     861045-37-6, Nicotinamide, N-[5-acetamido-2-(N-
IT
     acetylsulfanilyl)phenylsulfonyl]- 861045-77-4, Nicotinamide,
     N-(5-amino-2-sulfanilylphenylsulfonyl)-
        (preparation of)
RN
     861045-37-6 CAPLUS
CN
     Nicotinamide, N-[5-acetamido-2-(N-acetylsulfanilyl)phenylsulfonyl]- (4CI)
     (CA INDEX NAME)
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RN 861045-77-4 CAPLUS
CN Nicotinamide, N-(5-amino-2-sulfanilylphenylsulfonyl)- (4CI) (CA INDEX NAME)

$$H_2N$$
 $O = S = O$
 $O = O$
 H_2N
 $O = S$
 $O = O$
 O

L10 ANSWER 79 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1942:21515 CAPLUS

DN 36:21515

OREF 36:3323i,3324a

TI N-p-Toluenesulfonylpyridinecarboxamide

IN Frohring, William O.; Szabo, Lester J.; Landy, Maurice

PA S. M. A. Corp.

DT Patent

LA Unavailable

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
ΡI	US 2270201		19420113	US 1940-316228	19400129

AB This compound (suitable for use as a therapeutic agent in the treatment of infections of the coccus type) and the corresponding picolinoyl and isonicotinoyl amides are produced by a process which involves treating the acid amide with an aqueous solution of Na2CO3, adding p-toluenesulfonyl

chloride

thereto and treating with acetone to precipitate the amide.

RN 113513-61-4 CAPLUS

L10 ANSWER 80 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1942:21088 CAPLUS

DN 36:21088

OREF 36:3262a-b

TI Ocular absorption of sulfonamide derivatives after local application

AU P'an, Shih-Yi

Proceedings of the Society for Experimental Biology and Medicine (1942), 49, 384-6

CODEN: PSEBAA; ISSN: 0037-9727

DT Journal

LA Unavailable

AB cf. C. A. 35, 2215.8. The powdered compds. were placed in the eyes of rabbits. Sulfanilamide and N1-nicotinylsulfanilamide were absorbed in effective amts. by all tissues and fluids except the vitreous humor. Sulfapyridine and N1,N4-dinicotinylsulfanilamide were found in therapeutic concns. in the conjunctiva, cornea, sclera and aqueous humor. Sulfathiazole, sulfaguanidine and sulfadiazine were absorbed in effective concns. only by the conjunctiva and cornea.

RN 6005-34-1 CAPLUS

CN Nicotinamide, N-sulfanilyl- (8CI) (CA INDEX NAME)

RN 782502-22-1 CAPLUS

CN Sulfanilamide, N1, N4-bis(3-pyridylcarbonyl) - (4CI) (CA INDEX NAME)

L10 ANSWER 81 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1942:21087 CAPLUS

DN 36:21087

OREF 36:3261i,3262a

TI Drug prophylaxis against lethal effects of severe anoxia. II. Alcohol, amytal and pentobarbital

AU Emerson, George A.; Van Liere, E. J.; Morrison, James L.

Proceedings of the Society for Experimental Biology and Medicine (1942), 49, 376-9
CODEN: PSEBAA; ISSN: 0037-9727

DT Journal

LA Unavailable

AB cf. C. A. 34, 5938.1. Narcotic doses of EtOH reduced the lethal effects of acute anoxic anoxia in mice if administered 1 hr. previously. Amytal and pentobarbital did not produce comparable effects.

IT 6005-34-1, Nicotinamide, N-sulfanilyl-782502-22-1, Nicotinanilide, 4'-(3-pyridylcarbonylsulfamyl)(preparation of)

RN 6005-34-1 CAPLUS

CN Nicotinamide, N-sulfanilyl- (8CI) (CA INDEX NAME)

RN 782502-22-1 CAPLUS

CN Sulfanilamide, N1, N4-bis(3-pyridylcarbonyl) - (4CI) (CA INDEX NAME)

L10 ANSWER 82 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1940:24248 CAPLUS

DN 34:24248

OREF 34:3741i,3742a-c

TI N1,N4-Nicotinyl derivatives of sulfanilamide

AU Daniels, T. C.; Iwamoto, Harry

SO Journal of the American Chemical Society (1940), 62, 741-2 CODEN: JACSAT; ISSN: 0002-7863

DT Journal

LA Unavailable

Nicotinyl chloride and sulfanilamide in anhydrous C5H5N, refluxed 1 h., give AB 50-75% of N4-nicotinylsulfanilamide (I), m. 257-8°. Nicotinanilide (0.05 mol.), added to 0.5 mol. ClSO3H below 15° , the temperature gradually increased to 60°, maintained at this temperature for 2 h., the mixture cooled and treated with an excess of cold 28% NH4OH, gives 40-50% of I does not titrate to a phenolphthalein (II) end point. The N1-isomer (III) of I, prepared according to Crossley, Northey and Hultquist (C. A. 34, 392.8) also m. 257-8° but because of its greater acidity titrates quant. to a II end point. A 50% mixture of I and III m. 233-5°; titration shows that III does not rearrange during the melting. I and Ac20 give 50% of the N1-Ac derivative, m. 255-6°. I and nicotinyl chloride in C5H5N, refluxed 1 h., give 40% of N1,N4-dinicotinylsulfanilamide, m. 222°, resolidifies and then m. 248°; titration with NaOH of the higher-melting form gives the same equivalent weight as before melting. preliminary pharmacol. investigation indicates that I is effective in the treatment of exptl. hemolytic streptococcus infections and also certain types of pneumococcus infections. The toxicity of I is lower than that of either sulfanilamide or sulfapyridine.

IT 6005-34-1, Nicotinamide, N-sulfanilyl- 782502-22-1, Nicotinanilide, 4'-(3-pyridylcarbonylsulfamyl)(preparation of)

RN 6005-34-1 CAPLUS

CN Nicotinamide, N-sulfanilyl- (8CI) (CA INDEX NAME)

RN 782502-22-1 CAPLUS

CN Sulfanilamide, N1, N4-bis(3-pyridylcarbonyl) - (4CI) (CA INDEX NAME)

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L10 ANSWER 83 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
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AN 1940:2663 CAPLUS

DN 34:2663

OREF 34:392h-i,393a-i

- TI Sulfanilamide derivatives. IV. N1,N4-Diacylsulfanilamides and N1-acylsulfanilamides
- AU Crossley, M. L.; Northey, E. H.; Hultquist, Martin E.
- SO Journal of the American Chemical Society (1939), 61, 2950-5 CODEN: JACSAT; ISSN: 0002-7863
- DT Journal

solubility

- LA Unavailable
- AB cf. C. A. 32, 8382.6. The most generally applicable method for the synthesis of N1-acylsulfanilamides and that giving the best yield consists in the use of acyl halides and N4-acetylsulfanilamide (I) in C5H5N, followed by alkaline hydrolysis, the yield based on the halide averaging 60%. Acid anhydrides may also be used, Ac2O giving 60% of the di-Ac derivative, hydrolysis of which gives 32% of the N1-Ac derivative (solubility in H2O at

temperature, 0.9%). The N1-Na, derivative of I, prepared from I and NaOH with recrystn. from H2O and dehydration in vacuo at 60-70°, was used in earlier work but was discarded in favor of the C5H5N method. Dry fusion of I and acyl halides led in general to decomposition products together with the desired N1-acyl derivs. I and BzCl in PhMe, refluxed 20 h., give 40% of the N1-Bz derivative Attempts to prepare N1-alkyl-N1-acylsulfanilamides by hydrolysis of the corresponding N4-Ac derivs. resulted in complete hydrolysis of the N1-Ac derivative Such derivs. were prepared by acylating N-alkylnitrobenzenesulfonamides and reducing with Fe and AcOH in PhMe. In the series of derivs. of fatty acids, the lower members were moderately H2O-soluble; on ascending the series, the H2O solubility decreased and the

in fat solvents increased; H2O solubility of derivs. having chains of 12 C or more was less than 0.001 g./100 cc. All of the derivs. in which a H remained on the amide N formed very soluble Na salts, which were neutral for the lower members of the series but became increasingly alkaline for the higher members. All of these compds. could be titrated quant. to a phenolphthalein end-point, however, while sulfanilamide itself cannot be so titrated, since its Na salt is highly hydrolyzed at this pH. In general, the derivs. could be hydrolyzed quant. to the organic acid and the amide (or sulfanilic acid) by boiling with alc. HCl or more rapidly by heating to 180-200° with 65% H2SO4. The lower members of the series could be titrated quant. by diazotization of the N4-NH2 group. Alkylation of the N1-N gave derivs. which no longer formed salts with cations; these had increased solubility in organic solvents. These derivs.

were

sensitive to hydrolytic agents and in this resembled the N1-alkyldisulfanilamides (C. A. 32, 8382.3). In the tables of data qual. data are given for the solubility and the crystalline form. N1-Acylsulfanilamides:

Ac (II) m. 182-4°, propionyl m. 134-5°, butyryl m. 125.4-6.6°, isobutyryl m. 198.5-200°, 2-ethylbutyryl m. 189-93.5°, hexanoyl m. 129.2-9.9°, heptanoyl m. 121.8-3.6°, 2-ethylhexanoyl m. 165.5-8°, octanoyl m. 101-3°, decanoyl m. 119-21°, hexdecanoyl m. 112.5-14.5°, dodecanoyl (III) m. 127-8.5°, tetradecanoyl m. 113.5-17.7°, octadecanoyl m. 98-102°, 9-octadecenoyl, amorphous, hexahydrobenzoyl m. 198.5-200°, chaulmoogryl m. 97.9-9°, Bz m. 181.2-2.3°, p-nitrobenzoyl m. 235-40°, p-aminobenzoyl m. 197.8-9°, hydrocinnamoyl m. 160.3-1.5°,

cinnamoyl m. 130-3° and then 174-5°, 4'-carboxybenzoyl m. above 225° (decomposition), mandelyl m. 192.5-4.5° (decomposition), diphenylacetyl m. 210.5-12°, furoyl m. 191.5-2°, 2-phenylcinchoninyl m. 305-10°, nicotinyl m. 256-7.5°, 3-hydroxy-2-naphthoyl m. 245-50°. N1-Acetylmetanilamide, m. 153.5-5.5°; tetradecanoyl analog, m. 113.5-14.2°. N1-Methyl-N1-dodecanoylsulfanilamide, m. 59.3-60.5°. N1-Acyl derivs. of N4-acetylsulfanilamides: Ac m. 253.5-5°, propionyl m. 242.5-4.3°, isobutyryl m. 247-8°, butyryl 238.2-40°, isovaleryl m. 215-17.5°, 2-ethylbutyryl m. 270-2°, hexanoyl m. 191-3°, heptanoyl m. 205-7.5°, 2-ethylhexanoyl (IV), m. 214-15.6°, octanoyl m. 195-7.6°, decanoyl m. 143.2-4.8°, hendecanoyl m. 153.2-5°, dodecanoyl m. 130-6% tetradecanoyl m. 144.2-5°, 9-octadecanoyl m. 131-5°, chaulmoogryl, Bz m. 280-5°, hexahydrobenzoyl m. 210-22°, p-nitrobenzoyl m. 270-2°, p-aminobenzoyl m. 260-3°, hydrocinnamoyl m. 160° and then 202.8 -5.4°, cinnamoyl m. 228-9.5°, diphenylacetyl m. 248.5-51°, furoyl m. 240.5-41.5°, 2-phenylcinchoninyl m. 166-70°, nicotinyl m. 295-300°. N1,N4-Didodecanoylsulfanilamide, m. 144-5°, N1-dodecanoyl-N4-(N-acetylsulfanilyl)sulfanilamide, m. 120° and then 150-2°; N1-dodecanoyl-N2-sulfanilylsulfanilamide, m. $102-4^{\circ}$. The Na salt (with 1 mol H2O), NH4 and Et2NH2 salts of II and the Ag, Hg++ and Ca salts of III and the Na and Mg salts of IV were prepared and analyzed. Preliminary pharmacol. results indicate that III is effective in mice against infections by β -hemolytic streptococci and arrests the spread of tuberculous infections in cavies. 6005-34-1, Nicotinamide, N-sulfanilyl- 845960-39-6, Sulfanilamide, N4-acetyl-N1-3-pyridylcarbonyl-(preparation of) 6005-34-1 CAPLUS Nicotinamide, N-sulfanilyl- (8CI) (CA INDEX NAME)

IT

RN

CN

RN 845960-39-6 CAPLUS
CN Nicotinamide, N-(N-acetylsulfanilyl)- (5CI) (CA INDEX NAME)

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L8	156 S L6 SSS FUL SUB=L5
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- L11 ANSWER 1 OF 1 CAOLD COPYRIGHT 2006 ACS on STN
- AN CA52:10078b CAOLD
- TI N-oxides and related compds. - (VII) per-acid oxidation of conjugated pyridines
- Katritzky, A. R.; Monro, A. M. 114911-11-4 AU
- IT
- RN 114911-11-4 CAOLD
- Hydrazine, 1-nicotinoyl-1-(phenylsulfonyl)-, N-oxide (6CI) (CA INDEX CN

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